Heterolytic H_2 Activation Mediated by Low Coordinate L_3Fe-(μ-N)-FeL_3 Complexes to Generate Fe(μ-NH)(μ-H)Fe Species

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Supporting Information

I. Experimental Section

All manipulations were carried out using standard Schlenk or glove-box techniques under a dinitrogen atmosphere. Unless otherwise noted, solvents were deoxygenated and dried by thorough sparging with N_2 gas followed by passage through an activated alumina column. Non-halogenated solvents were tested with a standard purple solution of sodium benzophenone ketyl in tetrahydrofuran in order to confirm effective oxygen and moisture removal. All reagents were purchased from commercial vendors and used without further purification unless otherwise stated. The compounds $[([PhBP_3]Fe)_2N][Na(THF)_5]$ $\{\mathbf{1}\}\{Na(THF)_5\}$ and $\{\mathbf{1}\}^-$-(50% ^{15}N) were prepared according to literature procedures.[1] Elemental analyses were performed by Desert Analytics, Tucson, AZ. Deuterated THF and benzene were purchased from Cambridge Isotope Laboratories, Inc. and were degassed and dried over fine alumina (THF) or activated 3 Å molecular sieves (benzene) prior to use. A Varian Mercury-300 NMR spectrometer was used to record ^1H NMR and ^{31}P NMR spectra at ambient temperature. ^1H chemical shifts were referenced to residual solvent while ^{31}P chemical shifts were referenced to 85% H_3PO_4 at δ 0 ppm. ^{15}N NMR data were acquired on an Inova 500 MHz spectrometer and chemical shifts were referenced to CH_3NO_2 (380 ppm relative to liquid ammonia at 0 ppm). IR measurements were obtained as a Nujol mull using a Bio-Rad Excalibur FTS 3000 spectrometer controlled by Bio-Rad Merlin Software (v. 2.97) set at 4 cm^{-1} resolution. X-ray diffraction studies were carried out in the Beckman Institute Crystallographic Facility on a Bruker Smart 1000 CCD diffractometer.

EPR Measurements. X-band EPR spectra were obtained on a Bruker EMX spectrometer (controlled by Bruker Win EPR Software v. 3.0) equipped with a rectangular cavity working in the TE_{102} mode. Variable temperature measurements were conducted with an Oxford continuous-flow helium cryostat (temperature range 3.6 – 300 K). Accurate frequency values were provided by a frequency counter built into the microwave bridge. Solution spectra were acquired in 1-methyltetrahydrofuran. Sample preparation was performed under a dinitrogen atmosphere in an EPR tube equipped with a ground glass joint. EPR simulations were performed with the program WINEPR *SimFonia* (Version 1.25, Bruker Analytische Messtechnik GmbH).

Magnetic Measurements. Measurements were recorded using a Quantum Designs SQUID magnetometer running MPMSR2 software (Magnetic Property Measurement System Revision 2). Data were recorded at 5000 G. Samples were suspended in the magnetometer in a clear plastic straw sealed under nitrogen with Lilly No. 4 gel caps. Loaded samples were centered within the magnetometer using the DC centering scan at 35 K and 5000 G. Data were acquired at 2 – 10 K (one data point every 2 K), 10 – 60 K (one data point every 5 K), and 60 – 310 K (one data point every 10 K). The magnetic susceptibility was adjusted for diamagnetic contributions using the constitutive corrections of Pascal's constants. The molar magnetic susceptibility (χ_m) was calculated by converting the calculated magnetic susceptibility (χ) obtained from the magnetometer to a molar susceptibility (using the multiplication factor {(molecular weight)/[sample weight)*(field strength)]}). Effective magnetic moments were calculated using Equation 1. Solution magnetic moments were measured using Evans method.[2]

$$\mu_{eff} = \mathrm{sqrt}(7.997\ \chi_m T) \quad \text{(eqn. 1)}$$

[1] Brown, S. D.; Peters, J. C. *J. Am. Chem. Soc.* **2005,** *127,* 1913.
[2] (a) Sur, S. K. *J. Magn. Reson.* **1989,** *82,* 169. (b) Evans, D. F. *J. Chem. Soc.* **1959,** 2003.

Synthesis of [([PhBP$_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$], {**3**}{Na(THF)$_5$}**:** [([PhBP$_3$]Fe)$_2$(μ-N)][Na(THF)$_5$] ({**1**}{Na(THF)$_5$}, 0.203 g, 0.108 mmol) was dissolved in THF (20 mL) and transferred to a 100 mL sealed flask equipped with a stirbar. The resulting brown solution was frozen in liquid nitrogen and the N_2 atmosphere was evacuated and replaced with an atmosphere of H_2. The reaction was then allowed to warm to room temperature with stirring and within ten minutes had changed color from brown to green. After stirring for four hours at room temperature, volatiles were removed *in vacuo* and the crude solids were washed with benzene (3 x 30 mL), petroleum ether (2 x 20 mL), and dried to yield {**3**}{Na(THF)$_5$} as a green powder (0.175 g, 86%). X-ray quality crystals were grown via a THF/hexanes vapor diffusion chamber. ^{1}H NMR (THF-d_8, 300 MHz): δ 18.5 (s, 1H); 7.56 (d, J = 3.0 Hz, 4H); 7.03 (t, J = 7.2 Hz, 4H); 6.90 (m, 26H); 6.80 (t, J = 7.8 Hz, 12H); 6.56 (t, J = 7.8 Hz, 24H); 3.60 (m, 20H); 1.78 (m, 20H); 1.31 (br s, 12H). ^{31}P{^{1}H} NMR (THF-d_8, 121.4 MHz): δ 66.0 (s). Anal. Calcd. for $C_{110}H_{124}B_2Fe_2NNa0_5P_6$: C, 70.19; H, 6.64; N, 0.74 Found: C, 69.82; H, 6.50; N, 0.83. For the ^{15}N NMR data, a sample of {**1**}$^-$-50%^{15}N was hydrogenated in a J. Young tube. ^{15}N NMR (THF, 50.751 MHz): δ 406 (d, $J_{N\text{-}H}$ = 63 Hz). ^{1}H NMR (THF-d_8, 300 MHz): δ 18.5 (virtual triplet due to 50% ^{14}NH singlet and 50% ^{15}NH doublet with $J_{N\text{-}H}$ = 63 Hz, 1H).

Synthesis of ([PhBP$_3$]Fe)$_2$(μ-N), 2: [([PhBP$_3$]Fe)$_2$(μ-N)][Na(THF)$_5$] ({**1**}$^-${Na(THF)$_5$}, 0.300 g, 0.160 mmol) was dissolved in THF (20 mL) with stirring. A THF solution (5 mL) of PCl_3 (14 µL, 0.160 mmol) was added dropwise which resulted in a rapid darkening of the reaction solution. After 2 hours volatiles were removed under reduced pressure and the crude solids were extracted with benzene (50 mL), filtered over Celite, and lyophilized. The resulting solids were washed with Et_2O (2 x 20 mL) and dried to obtain **2** as a dark solid (0.157 g, 66%). X-ray quality crystals were grown via vapor diffusion of petroleum ether into a THF solution. ^{1}H NMR (C_6D_6, 300 MHz): δ 52.5 (s); 19.7 (s); 12.6 (s); 11.5 (t, J = 6.0 Hz); 6.14 (d, J = 6.0 Hz); -1.69 (s); -6.44 (s). μ_{eff} = 2.3 μ_B at 50 K (SQUID). Anal. Calcd. for $C_{90}H_{82}B_2Fe_2NP_6$: C, 72.22; H, 5.52; N, 0.94 Found: C, 71.92; H, 5.56; N, 0.74.

Synthesis of ([PhBP$_3$]Fe)$_2$(μ-NH)(μ-H), 4: [([PhBP$_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$] ({**3**}{Na(THF)$_5$}, 0.400 g, 0.213 mmol) was dissolved in THF (40 mL) with stirring. Solid [NO][BF_4] (0.0248 g, 0.213 mmol) was added to this solution in one portion. The green color of {**3**}{Na(THF)$_5$} gradually fades and after two hours volatiles were removed under reduced pressure and the crude solids were extracted with benzene (~ 80 mL), filtered over Celite, and lyophilized. The resulting solids were washed with Et_2O (2 x 20 mL) and dried to obtain **4** as a dark solid (0.248 g, 78%). ^{1}H NMR (THF-d_8, 300 MHz): δ 21.4 (v br, s); 11.9 (s); 9.00 (s); 8.51 (t, J = 6.3 Hz); 7.11 (s); 3.53 (s, overlaps with residual solvent resonance); 1.03 (br, s). μ_{eff} = 2.2 μ_B at 50 K (SQUID). IR (Nujol): ν_{NH} = 3319 cm^{-1}. Anal. Calcd. for $C_{90}H_{84}B_2Fe_2NP_6$: C, 72.12; H, 5.65; N, 0.93 Found: C, 71.73; H, 5.76; N, 0.80.

Figure 1. EPR spectrum of **2** (MeTHF at 4 K, X-band, 9.378 GHz). A trace impurity is also evident at ca. $g = 10.1$.

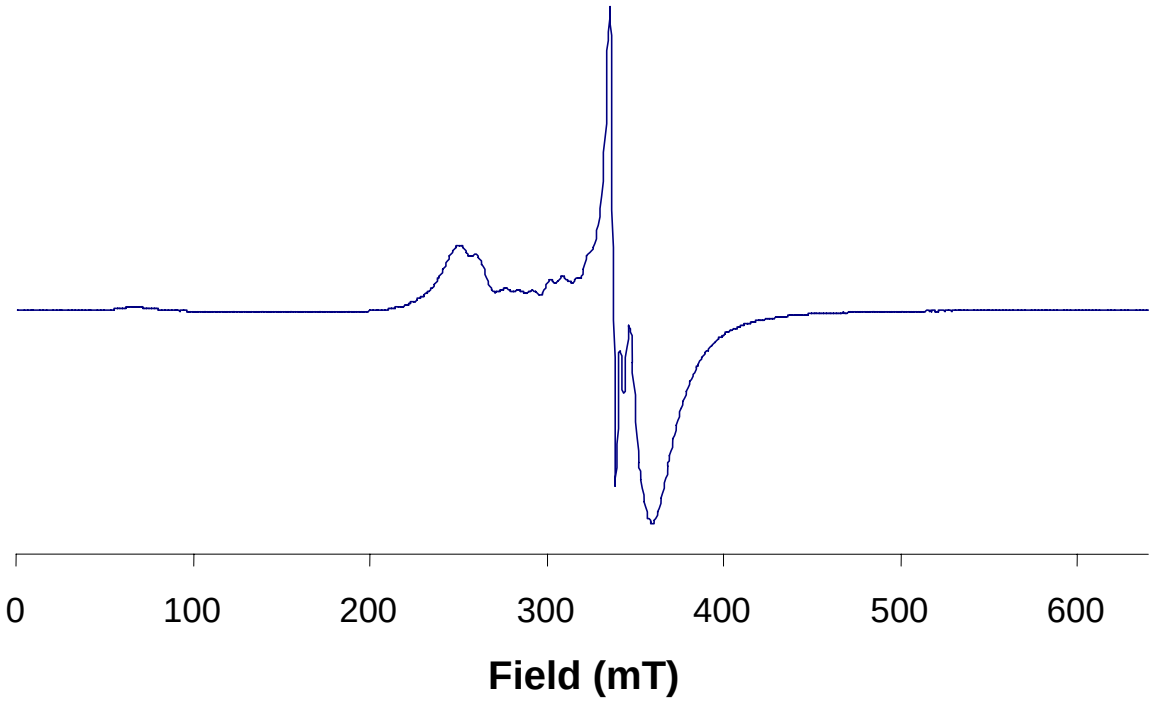

Figure 2. EPR spectrum of **4** (MeTHF at 20 K, X-band, 9.374 GHz).

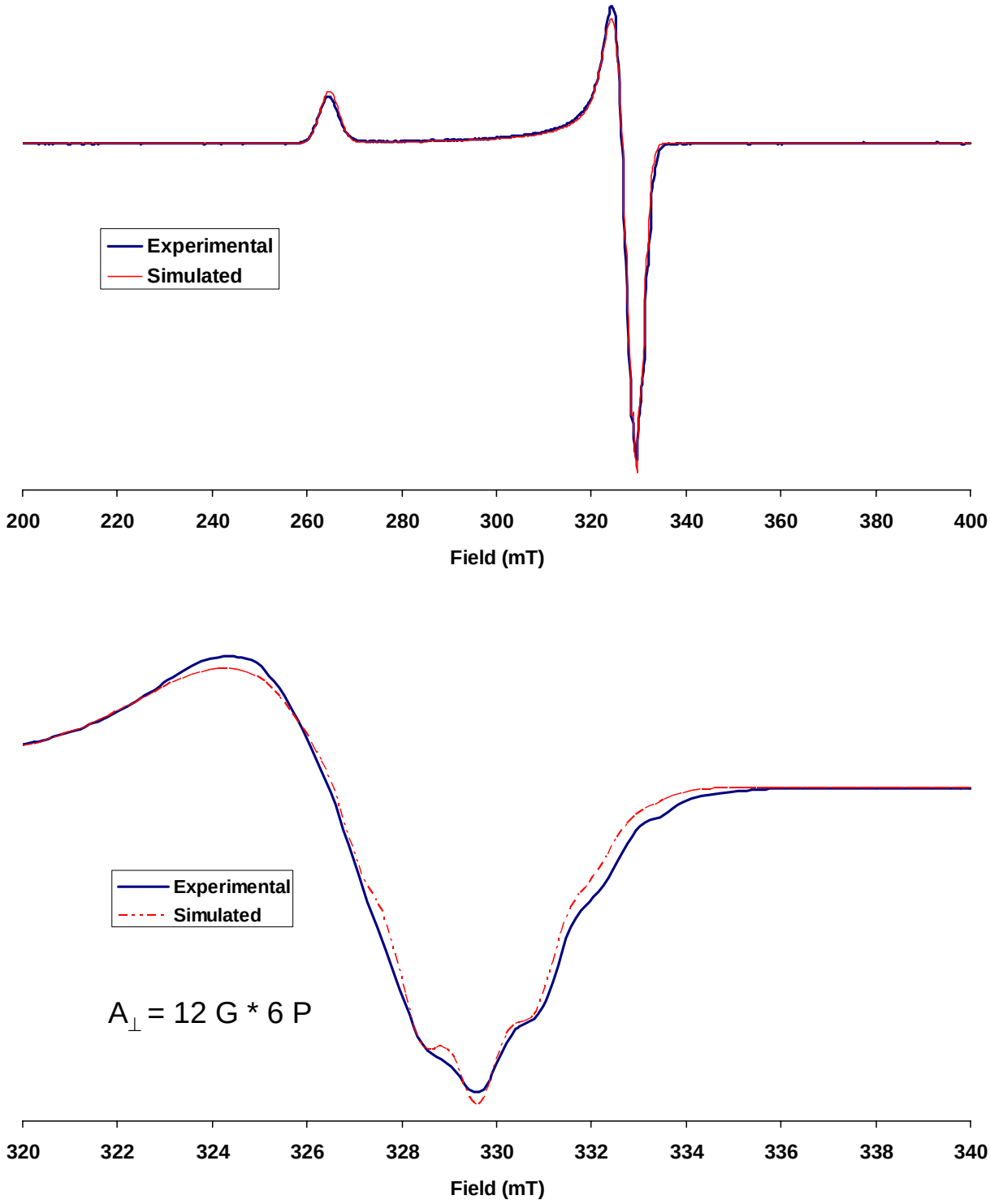

Figure 3. SQUID data for **2**.

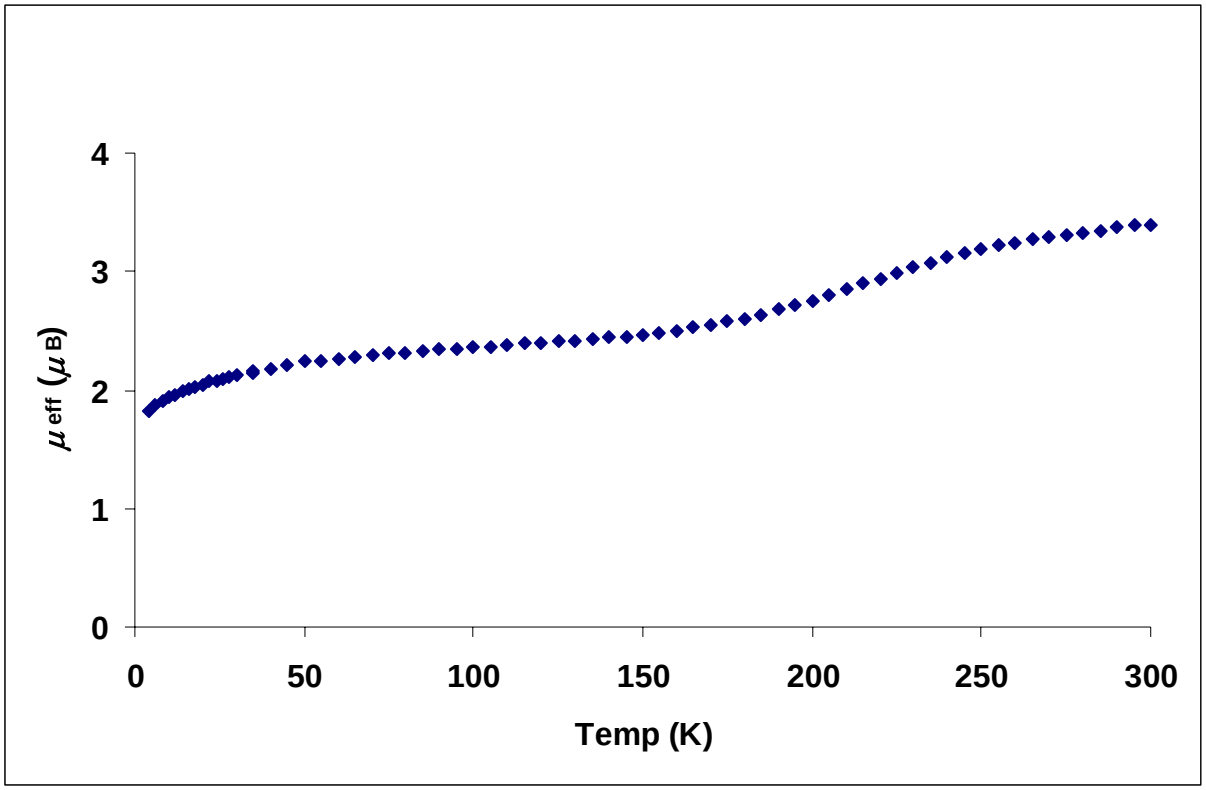

Figure 4. SQUID data for **4**.

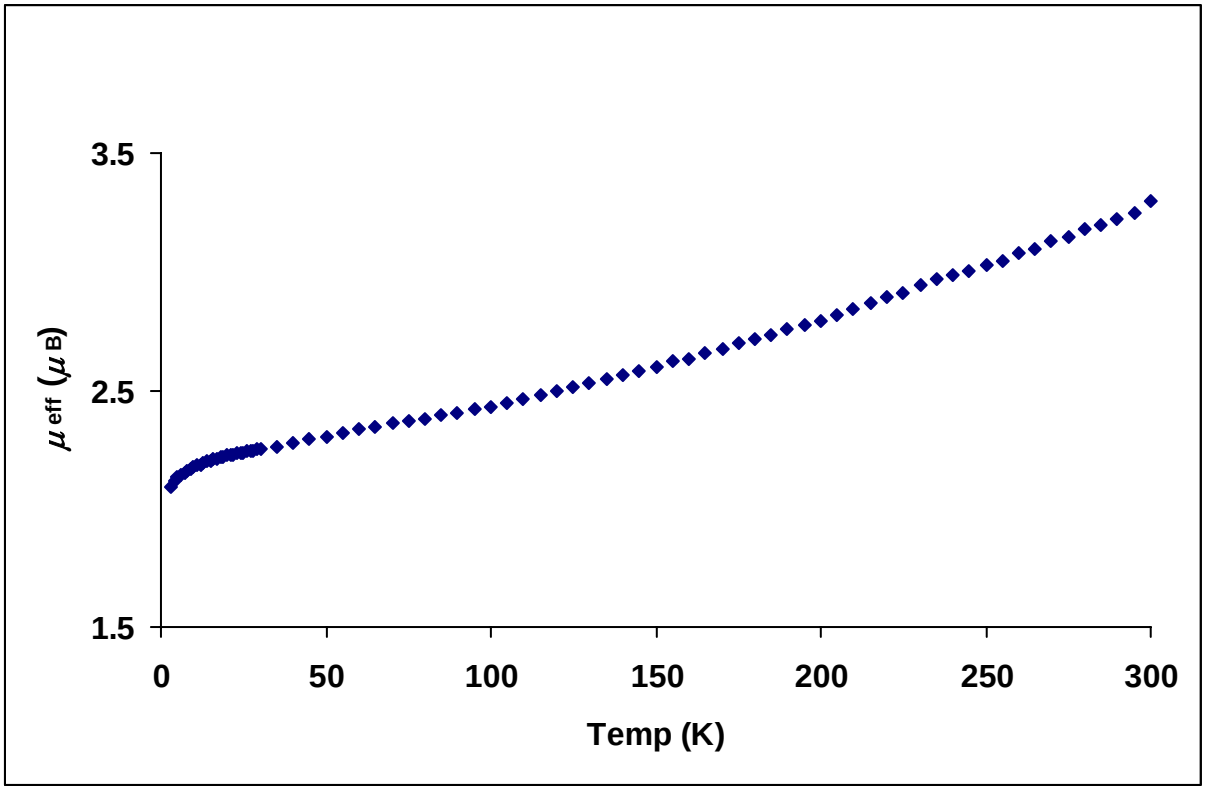

Figure 5. Optical data for {**1**}$^{-}$ and **2**.

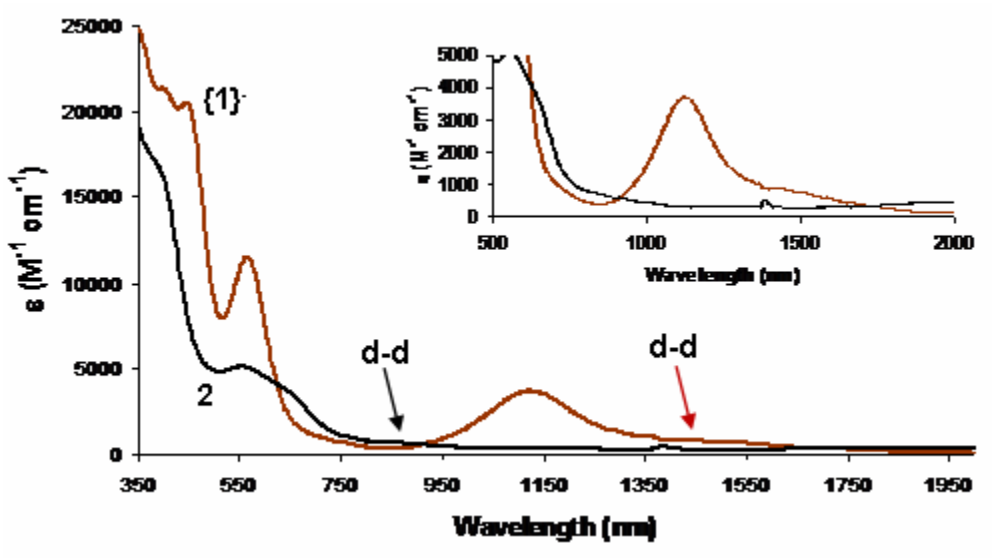

Figure 6. Optical data for {**3**}$^{-}$ and **4**.

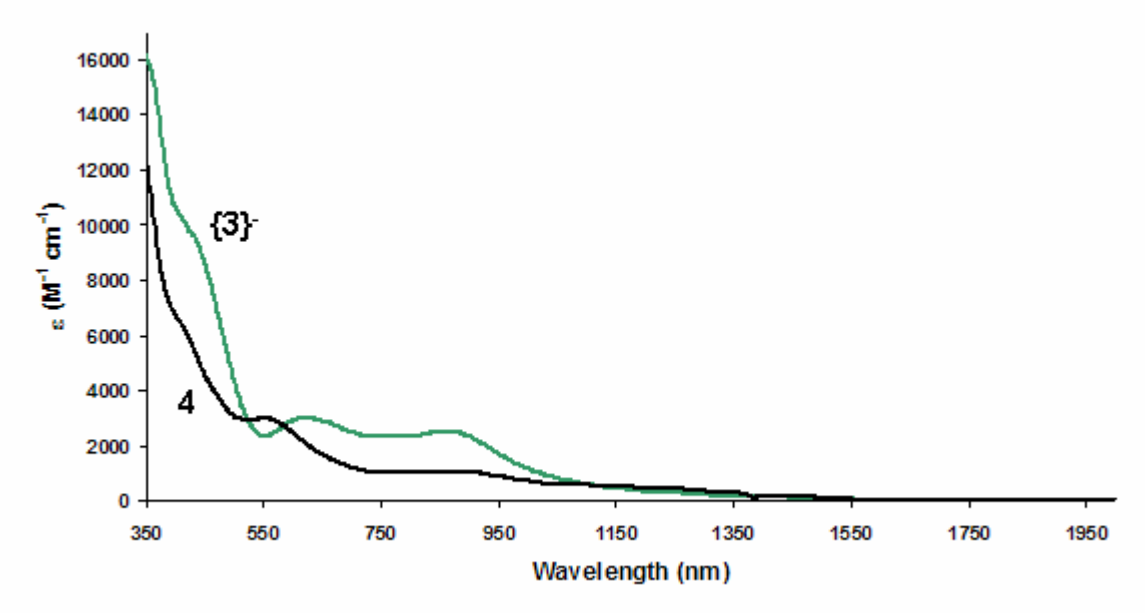

Figure 7. Core-labeled drawing of $[([PhBP_3]Fe)_2(\mu\text{-NH})(\mu\text{-H})][Na(THF)_5]$, $\{\mathbf{3}\}\{Na(THF)_5\}$. Hydrogen atoms have been omitted for clarity.

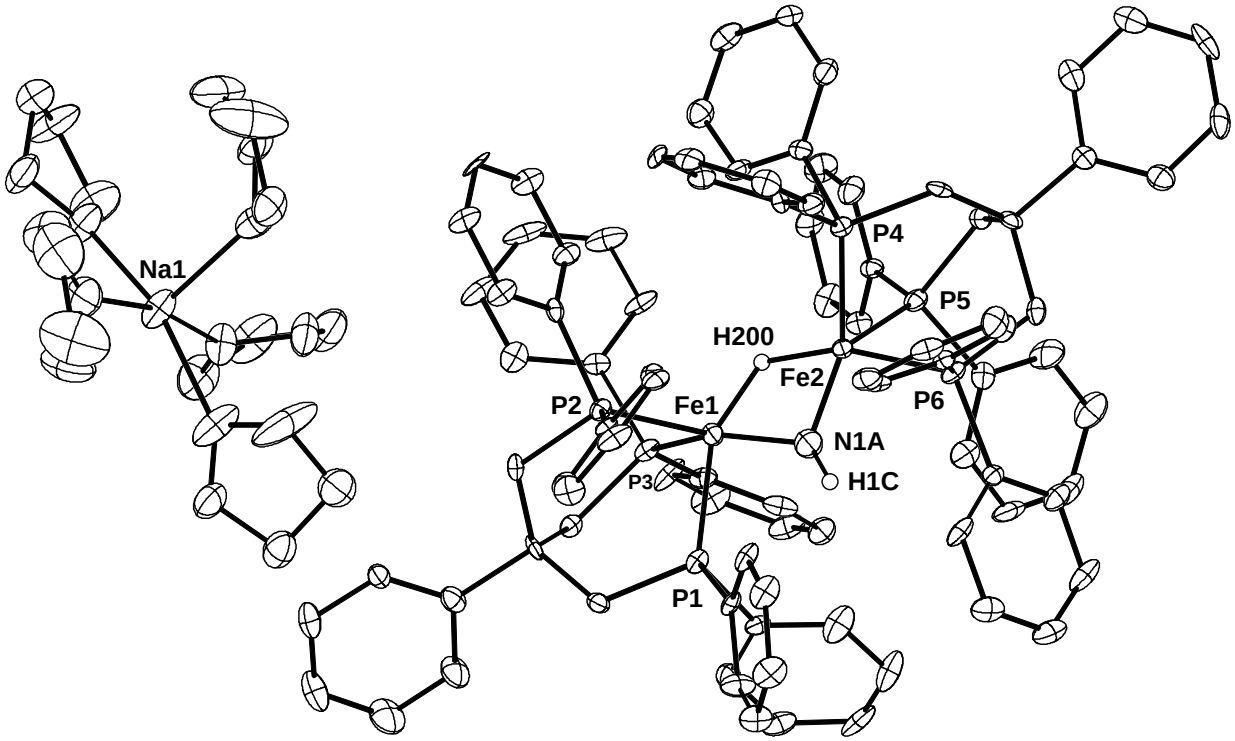

Figure 8. Core-labeled drawing of ([$PhBP_3$]Fe)$_2$(μ-N), **2**. Hydrogen atoms and two THF solvent molecules have been omitted for clarity.

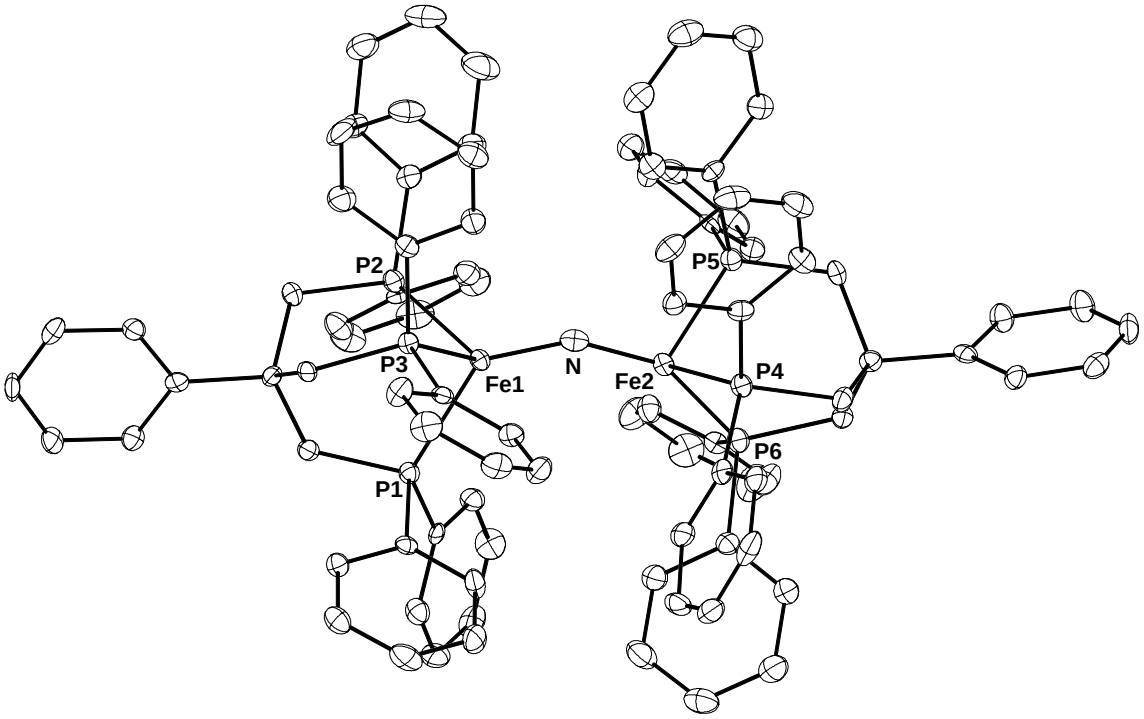

Table 1. Crystal data and structure refinement for [([$PhBP_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$].

Empirical formula	$C_{90}H_{84}B_2Fe_2NP_6 \bullet C_{20}H_{40}NaO_5$
Formula weight	1882.23
Crystallization Solvent	THF/Hexanes
Crystal Habit	Blade
Crystal size	0.28 x 0.17 x 0.16 mm^3
Crystal color	Brown

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 12381 reflections used in lattice determination	2.21 to 28.29°
Unit cell dimensions	a = 13.712(2) Å b = 23.001(4) Å β= 91.006(6)° c = 30.221(5) Å
Volume	9530(3) Å^3
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.312 Mg/m^3
F(000)	3976
θ range for data collection	1.11 to 29.08°
Completeness to θ = 29.08°	91.1 %
Index ranges	$-18 \le h \le 18$, $-31 \le k \le 30$, $-40 \le l \le 39$
Data collection scan type	ω scans at 7 ϕ settings
Reflections collected	86544
Independent reflections	23261 [R_{int}= 0.1409]
Absorption coefficient	0.466 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9292 and 0.8807

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	23261 / 12 / 1163
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.157
Final R indices [$I>2\sigma(I)$, 9380 reflections]	R1 = 0.0666, *w*R2 = 0.0941
R indices (all data)	R1 = 0.2064, *w*R2 = 0.1092
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.113
Average shift/error	0.000
Largest diff. peak and hole	0.733 and -0.688 e.Å^{-3}

Special Refinement Details

Restraints were placed on C99 to force its anisotropic displacement parameter to tend toward isotropic behavior. The amide-hydride bridge between Fe1and Fe2 is disordered and the minor bridge component was refined to be flat. Additionally, the hydride to Fe distances were refined but restrained to be equal.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for [([$PhBP_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$]. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Fe(1)	2484(1)	4089(1)	2102(1)	16(1)	1
Fe(2)	2567(1)	4170(1)	2979(1)	14(1)	1
N(1A)	1736(5)	3883(3)	2571(2)	49(2)	0.703(7)
N(1B)	3479(11)	4044(1)	2530(3)	27(4)	0.297(7)
P(1)	1452(1)	3564(1)	1697(1)	14(1)	1
P(2)	2205(1)	4830(1)	1656(1)	14(1)	1
P(3)	3711(1)	3823(1)	1672(1)	16(1)	1
P(4)	2764(1)	5009(1)	3336(1)	13(1)	1
P(5)	3765(1)	3817(1)	3410(1)	15(1)	1
P(6)	1493(1)	3902(1)	3491(1)	15(1)	1
B(1)	2387(4)	4016(2)	908(1)	15(1)	1
B(2)	2828(4)	4341(2)	4159(2)	14(1)	1
C(21)	1420(3)	3677(2)	1098(1)	15(1)	1
C(22)	3390(3)	3684(2)	1095(1)	14(1)	1
C(23)	2374(3)	4695(2)	1066(1)	13(1)	1
C(24)	2515(3)	4970(2)	3930(1)	15(1)	1
C(25)	3864(3)	4124(2)	3963(1)	15(1)	1
C(26)	1990(3)	3849(2)	4047(1)	15(1)	1
C(27)	2379(3)	3968(2)	365(1)	19(1)	1
C(28)	2391(3)	4441(2)	83(1)	18(1)	1
C(29)	2369(3)	4407(2)	-380(1)	28(1)	1
C(30)	2357(3)	3863(2)	-570(2)	33(1)	1
C(31)	2360(4)	3379(2)	-307(2)	38(1)	1
C(32)	2366(3)	3428(2)	153(1)	29(1)	1
C(33)	130(3)	3566(2)	1802(1)	13(1)	1
C(34)	-324(3)	3998(2)	2042(1)	19(1)	1
C(35)	-1340(3)	4013(2)	2078(1)	21(1)	1
C(36)	-1905(3)	3591(2)	1888(2)	25(1)	1
C(37)	-1467(3)	3157(2)	1657(1)	24(1)	1
C(38)	-466(3)	3134(2)	1617(1)	23(1)	1
C(39)	1639(3)	2778(2)	1780(1)	15(1)	1
C(40)	1989(3)	2400(2)	1465(1)	19(1)	1
C(41)	2100(3)	1805(2)	1555(2)	24(1)	1
C(42)	1834(3)	1591(2)	1956(2)	28(1)	1
C(43)	1472(3)	1954(2)	2276(2)	30(1)	1
C(44)	1378(3)	2542(2)	2182(2)	29(1)	1
C(45)	4783(3)	4307(2)	1636(1)	14(1)	1
C(46)	5005(3)	4619(2)	1252(1)	22(1)	1
C(47)	5844(3)	4968(2)	1239(2)	29(1)	1
C(48)	6453(3)	5002(2)	1603(2)	30(1)	1
C(49)	6246(3)	4692(2)	1982(2)	28(1)	1
C(50)	5422(3)	4357(2)	2000(2)	22(1)	1
C(51)	4386(3)	3153(2)	1819(1)	17(1)	1
C(52)	5256(3)	3021(2)	1617(2)	26(1)	1
C(53)	5747(3)	2510(2)	1718(2)	29(1)	1
C(54)	5367(3)	2114(2)	2013(2)	27(1)	1
C(55)	4504(3)	2235(2)	2213(1)	24(1)	1
C(56)	4018(3)	2756(2)	2120(1)	22(1)	1

C(57)	954(3)	5107(2)	1700(1)	13(1)	1
C(58)	253(3)	5089(2)	1364(1)	20(1)	1
C(59)	-670(3)	5343(2)	1419(2)	23(1)	1
C(60)	-884(3)	5620(2)	1807(2)	22(1)	1
C(61)	-195(3)	5645(2)	2143(1)	18(1)	1
C(62)	707(3)	5390(2)	2093(1)	16(1)	1
C(63)	2826(3)	5547(2)	1710(1)	12(1)	1
C(64)	2375(3)	6050(2)	1537(1)	21(1)	1
C(65)	2849(3)	6579(2)	1556(1)	22(1)	1
C(66)	3793(3)	6623(2)	1729(1)	23(1)	1
C(67)	4247(3)	6127(2)	1895(1)	26(1)	1
C(68)	3760(3)	5595(2)	1885(1)	17(1)	1
C(69)	2091(3)	5677(2)	3159(1)	12(1)	1
C(70)	1214(3)	5830(2)	3347(1)	19(1)	1
C(71)	720(3)	6339(2)	3224(1)	22(1)	1
C(72)	1107(3)	6699(2)	2910(1)	21(1)	1
C(73)	1999(3)	6549(2)	2714(1)	20(1)	1
C(74)	2467(3)	6046(2)	2837(1)	18(1)	1
C(75)	4002(3)	5323(2)	3308(1)	14(1)	1
C(76)	4420(3)	5655(2)	3642(1)	21(1)	1
C(77)	5336(3)	5908(2)	3591(1)	23(1)	1
C(78)	5817(3)	5841(2)	3201(2)	23(1)	1
C(79)	5406(3)	5525(2)	2865(2)	22(1)	1
C(80)	4511(3)	5254(2)	2923(1)	20(1)	1
C(81)	5052(3)	3792(2)	3228(1)	14(1)	1
C(82)	5722(3)	4226(2)	3331(1)	22(1)	1
C(83)	6678(3)	4190(2)	3202(1)	26(1)	1
C(84)	7008(3)	3722(2)	2966(1)	23(1)	1
C(85)	6361(3)	3283(2)	2852(1)	22(1)	1
C(86)	5398(3)	3323(2)	2979(1)	20(1)	1
C(87)	3646(3)	3020(2)	3504(1)	18(1)	1
C(88)	4159(3)	2742(2)	3846(2)	32(1)	1
C(89)	4156(3)	2145(2)	3882(2)	32(1)	1
C(90)	3640(4)	1821(2)	3568(2)	28(1)	1
C(91)	3142(3)	2079(2)	3238(2)	26(1)	1
C(92)	3135(3)	2686(2)	3207(1)	23(1)	1
C(93)	764(3)	3224(2)	3405(1)	14(1)	1
C(94)	1030(3)	2708(2)	3627(1)	20(1)	1
C(95)	499(3)	2198(2)	3550(2)	26(1)	1
C(96)	-277(3)	2188(2)	3252(2)	26(1)	1
C(97)	-546(3)	2701(2)	3043(1)	23(1)	1
C(98)	-16(3)	3207(2)	3119(1)	22(1)	1
C(99)	436(3)	4395(2)	3545(1)	13(1)	1
C(100)	16(3)	4527(2)	3952(1)	19(1)	1
C(101)	-794(3)	4890(2)	3970(2)	24(1)	1
C(102)	-1207(3)	5109(2)	3588(2)	19(1)	1
C(103)	-801(3)	4989(2)	3189(2)	21(1)	1
C(104)	33(3)	4639(2)	3170(1)	19(1)	1
C(105)	2456(3)	4170(2)	5023(1)	21(1)	1
C(106)	2571(3)	4306(2)	5470(1)	24(1)	1
C(107)	3200(3)	4740(2)	5609(1)	26(1)	1
C(108)	3714(3)	5031(2)	5293(2)	27(1)	1
C(109)	3596(3)	4902(2)	4847(1)	24(1)	1
C(110)	2950(3)	4462(2)	4693(1)	15(1)	1

Na(1)	2544(1)	7279(1)	-155(1)	36(1)	1
O(1)	1212(2)	6632(1)	-169(1)	51(1)	1
O(2)	1505(3)	8030(2)	-417(1)	44(1)	1
O(3)	4069(2)	7699(1)	-338(1)	43(1)	1
O(4)	3473(2)	6442(1)	-17(1)	34(1)	1
O(5)	2407(2)	7577(1)	577(1)	37(1)	1
C(1)	554(5)	6582(2)	199(2)	90(3)	1
C(2)	413(4)	5946(2)	262(2)	51(2)	1
C(3)	455(3)	5710(2)	-203(2)	37(1)	1
C(4)	1193(4)	6103(2)	-425(2)	44(2)	1
C(5)	617(5)	7898(2)	-649(2)	66(2)	1
C(6)	-135(5)	8320(3)	-497(2)	96(2)	1
C(7)	456(5)	8832(3)	-338(2)	75(2)	1
C(8)	1519(4)	8649(2)	-396(2)	59(2)	1
C(9)	1592(4)	7912(2)	737(2)	39(1)	1
C(10)	2022(4)	8496(3)	883(2)	93(2)	1
C(11)	3097(4)	8458(3)	758(2)	63(2)	1
C(12)	3291(4)	7830(2)	758(2)	42(2)	1
C(13)	4158(4)	8287(2)	-479(2)	45(2)	1
C(14)	5046(4)	8500(2)	-233(2)	47(2)	1
C(15)	5738(4)	7988(2)	-261(2)	58(2)	1
C(16)	5047(4)	7470(2)	-271(2)	58(2)	1
C(17)	3405(4)	6195(2)	414(2)	42(2)	1
C(18)	4307(4)	5825(2)	487(2)	53(2)	1
C(19)	4869(4)	5877(2)	71(2)	56(2)	1
C(20)	4106(4)	6073(2)	-263(2)	54(2)	1

Table 3. Bond lengths [Å] and angles [°] for [([$PhBP_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$].

Fe(1)-H(201)	1.508(14)	C(22)-H(22B)	0.9900
Fe(1)-H(200)	1.508(14)	C(23)-H(23A)	0.9900
Fe(1)-N(1A)	1.826(5)	C(23)-H(23B)	0.9900
Fe(1)-N(1B)	1.868(12)	C(24)-H(24A)	0.9900
Fe(1)-P(2)	2.2024(13)	C(24)-H(24B)	0.9900
Fe(1)-P(1)	2.2121(13)	C(25)-H(25A)	0.9900
Fe(1)-P(3)	2.2274(13)	C(25)-H(25B)	0.9900
Fe(1)-Fe(2)	2.6595(9)	C(26)-H(26A)	0.9900
Fe(1)-H(200)	1.508(14)	C(26)-H(26B)	0.9900
Fe(1)-H(201)	1.508(14)	C(27)-C(28)	1.382(5)
Fe(2)-H(200)	1.508(14)	C(27)-C(32)	1.397(5)
Fe(2)-H(201)	1.508(14)	C(28)-C(29)	1.402(5)
Fe(2)-N(1A)	1.790(5)	C(28)-H(28)	0.9500
Fe(2)-N(1B)	1.883(14)	C(29)-C(30)	1.376(6)
Fe(2)-P(4)	2.2247(13)	C(29)-H(29)	0.9500
Fe(2)-P(5)	2.2306(13)	C(30)-C(31)	1.368(6)
Fe(2)-P(6)	2.2411(13)	C(30)-H(30)	0.9500
Fe(2)-H(200)	1.508(14)	C(31)-C(32)	1.393(6)
Fe(2)-H(201)	1.508(14)	C(31)-H(31)	0.9500
N(1A)-H(1C)	0.8800	C(32)-H(32)	0.9500
N(1A)-H(201)	0.774(12)	C(33)-C(34)	1.385(5)
N(1B)-H(200)	0.81(5)	C(33)-C(38)	1.397(5)
N(1B)-H(1D)	0.8800	C(34)-C(35)	1.400(5)
P(1)-C(21)	1.826(4)	C(34)-H(34)	0.9500
P(1)-C(39)	1.842(4)	C(35)-C(36)	1.362(5)
P(1)-C(33)	1.847(4)	C(35)-H(35)	0.9500
P(2)-C(23)	1.830(4)	C(36)-C(37)	1.364(5)
P(2)-C(57)	1.838(4)	C(36)-H(36)	0.9500
P(2)-C(63)	1.861(4)	C(37)-C(38)	1.381(5)
P(3)-C(22)	1.822(4)	C(37)-H(37)	0.9500
P(3)-C(51)	1.848(4)	C(38)-H(38)	0.9500
P(3)-C(45)	1.849(4)	C(39)-C(40)	1.380(5)
P(4)-C(24)	1.834(4)	C(39)-C(44)	1.384(5)
P(4)-C(75)	1.848(4)	C(40)-C(41)	1.404(5)
P(4)-C(69)	1.865(4)	C(40)-H(40)	0.9500
P(5)-C(25)	1.817(4)	C(41)-C(42)	1.364(5)
P(5)-C(81)	1.858(4)	C(41)-H(41)	0.9500
P(5)-C(87)	1.864(4)	C(42)-C(43)	1.378(6)
P(6)-C(26)	1.806(4)	C(42)-H(42)	0.9500
P(6)-C(99)	1.849(4)	C(43)-C(44)	1.389(5)
P(6)-C(93)	1.869(4)	C(43)-H(43)	0.9500
B(1)-C(23)	1.632(6)	C(44)-H(44)	0.9500
B(1)-C(27)	1.647(6)	C(45)-C(50)	1.398(5)
B(1)-C(21)	1.651(6)	C(45)-C(46)	1.402(5)
B(1)-C(22)	1.662(6)	C(46)-C(47)	1.404(6)
B(2)-C(25)	1.628(6)	C(46)-H(46)	0.9500
B(2)-C(110)	1.644(6)	C(47)-C(48)	1.371(6)
B(2)-C(26)	1.645(6)	C(47)-H(47)	0.9500
B(2)-C(24)	1.657(6)	C(48)-C(49)	1.383(6)
C(21)-H(21A)	0.9900	C(48)-H(48)	0.9500
C(21)-H(21B)	0.9900	C(49)-C(50)	1.370(5)
C(22)-H(22A)	0.9900	C(49)-H(49)	0.9500

C(50)-H(50)	0.9500	C(79)-H(79)	0.9500
C(51)-C(52)	1.383(5)	C(80)-H(80)	0.9500
C(51)-C(56)	1.391(5)	C(81)-C(82)	1.388(5)
C(52)-C(53)	1.385(6)	C(81)-C(86)	1.402(5)
C(52)-H(52)	0.9500	C(82)-C(83)	1.376(5)
C(53)-C(54)	1.382(6)	C(82)-H(82)	0.9500
C(53)-H(53)	0.9500	C(83)-C(84)	1.373(6)
C(54)-C(55)	1.368(6)	C(83)-H(83)	0.9500
C(54)-H(54)	0.9500	C(84)-C(85)	1.383(5)
C(55)-C(56)	1.398(5)	C(84)-H(84)	0.9500
C(55)-H(55)	0.9500	C(85)-C(86)	1.386(5)
C(56)-H(56)	0.9500	C(85)-H(85)	0.9500
C(57)-C(58)	1.386(5)	C(86)-H(86)	0.9500
C(57)-C(62)	1.400(5)	C(87)-C(92)	1.367(5)
C(58)-C(59)	1.408(5)	C(87)-C(88)	1.394(6)
C(58)-H(58)	0.9500	C(88)-C(89)	1.378(6)
C(59)-C(60)	1.370(5)	C(88)-H(88)	0.9500
C(59)-H(59)	0.9500	C(89)-C(90)	1.390(6)
C(60)-C(61)	1.376(5)	C(89)-H(89)	0.9500
C(60)-H(60)	0.9500	C(90)-C(91)	1.339(6)
C(61)-C(62)	1.379(5)	C(90)-H(90)	0.9500
C(61)-H(61)	0.9500	C(91)-C(92)	1.399(6)
C(62)-H(62)	0.9500	C(91)-H(91)	0.9500
C(63)-C(68)	1.381(5)	C(92)-H(92)	0.9500
C(63)-C(64)	1.409(5)	C(93)-C(98)	1.364(5)
C(64)-C(65)	1.379(5)	C(93)-C(94)	1.408(5)
C(64)-H(64)	0.9500	C(94)-C(95)	1.399(5)
C(65)-C(66)	1.393(6)	C(94)-H(94)	0.9500
C(65)-H(65)	0.9500	C(95)-C(96)	1.381(6)
C(66)-C(67)	1.387(5)	C(95)-H(95)	0.9500
C(66)-H(66)	0.9500	C(96)-C(97)	1.385(6)
C(67)-C(68)	1.395(5)	C(96)-H(96)	0.9500
C(67)-H(67)	0.9500	C(97)-C(98)	1.390(5)
C(68)-H(68)	0.9500	C(97)-H(97)	0.9500
C(69)-C(70)	1.384(5)	C(98)-H(98)	0.9500
C(69)-C(74)	1.398(5)	C(99)-C(104)	1.373(5)
C(70)-C(71)	1.400(5)	C(99)-C(100)	1.401(5)
C(70)-H(70)	0.9500	C(100)-C(101)	1.392(5)
C(71)-C(72)	1.374(5)	C(100)-H(100)	0.9500
C(71)-H(71)	0.9500	C(101)-C(102)	1.374(5)
C(72)-C(73)	1.410(5)	C(101)-H(101)	0.9500
C(72)-H(72)	0.9500	C(102)-C(103)	1.366(5)
C(73)-C(74)	1.371(5)	C(102)-H(102)	0.9500
C(73)-H(73)	0.9500	C(103)-C(104)	1.399(5)
C(74)-H(74)	0.9500	C(103)-H(103)	0.9500
C(75)-C(80)	1.378(5)	C(104)-H(104)	0.9500
C(75)-C(76)	1.381(5)	C(105)-C(110)	1.390(5)
C(76)-C(77)	1.396(5)	C(105)-C(106)	1.393(5)
C(76)-H(76)	0.9500	C(105)-H(105)	0.9500
C(77)-C(78)	1.368(5)	C(106)-C(107)	1.381(6)
C(77)-H(77)	0.9500	C(106)-H(106)	0.9500
C(78)-C(79)	1.364(5)	C(107)-C(108)	1.370(6)
C(78)-H(78)	0.9500	C(107)-H(107)	0.9500
C(79)-C(80)	1.390(5)	C(108)-C(109)	1.389(5)

C(108)-H(108)	0.9500	C(14)-C(15)	1.516(6)
C(109)-C(110)	1.418(6)	C(14)-H(14A)	0.9900
C(109)-H(109)	0.9500	C(14)-H(14B)	0.9900
Na(1)-O(5)	2.325(4)	C(15)-C(16)	1.523(6)
Na(1)-O(4)	2.341(3)	C(15)-H(15A)	0.9900
Na(1)-O(1)	2.356(4)	C(15)-H(15B)	0.9900
Na(1)-O(2)	2.368(4)	C(16)-H(16A)	0.9900
Na(1)-O(3)	2.379(4)	C(16)-H(16B)	0.9900
O(1)-C(4)	1.442(5)	C(17)-C(18)	1.514(6)
O(1)-C(1)	1.449(6)	C(17)-H(17A)	0.9900
O(2)-C(5)	1.426(6)	C(17)-H(17B)	0.9900
O(2)-C(8)	1.426(5)	C(18)-C(19)	1.492(7)
O(3)-C(13)	1.423(5)	C(18)-H(18A)	0.9900
O(3)-C(16)	1.451(6)	C(18)-H(18B)	0.9900
O(4)-C(17)	1.424(5)	C(19)-C(20)	1.511(7)
O(4)-C(20)	1.433(5)	C(19)-H(19A)	0.9900
O(5)-C(12)	1.444(5)	C(19)-H(19B)	0.9900
O(5)-C(9)	1.448(5)	C(20)-H(20A)	0.9900
C(1)-C(2)	1.488(7)	C(20)-H(20B)	0.9900
C(1)-H(1A)	0.9900		
C(1)-H(1B)	0.9900	H(201)-Fe(1)-H(200)	54.0(19)
C(2)-C(3)	1.508(6)	H(201)-Fe(1)-N(1A)	24.6(4)
C(2)-H(2A)	0.9900	H(200)-Fe(1)-N(1A)	70.3(10)
C(2)-H(2B)	0.9900	H(201)-Fe(1)-N(1B)	73.3(11)
C(3)-C(4)	1.522(6)	H(200)-Fe(1)-N(1B)	25(2)
C(3)-H(3A)	0.9900	N(1A)-Fe(1)-N(1B)	82.0(4)
C(3)-H(3B)	0.9900	H(201)-Fe(1)-P(2)	111.5(5)
C(4)-H(4A)	0.9900	H(200)-Fe(1)-P(2)	114(2)
C(4)-H(4B)	0.9900	N(1A)-Fe(1)-P(2)	125.5(2)
C(5)-C(6)	1.494(7)	N(1B)-Fe(1)-P(2)	125.65(12)
C(5)-H(5A)	0.9900	H(201)-Fe(1)-P(1)	106.4(8)
C(5)-H(5B)	0.9900	H(200)-Fe(1)-P(1)	153.5(16)
C(6)-C(7)	1.502(8)	N(1A)-Fe(1)-P(1)	85.77(18)
C(6)-H(6A)	0.9900	N(1B)-Fe(1)-P(1)	143.74(5)
C(6)-H(6B)	0.9900	P(2)-Fe(1)-P(1)	88.98(5)
C(7)-C(8)	1.530(7)	H(201)-Fe(1)-P(3)	153.2(9)
C(7)-H(7A)	0.9900	H(200)-Fe(1)-P(3)	102.5(15)
C(7)-H(7B)	0.9900	N(1A)-Fe(1)-P(3)	145.2(2)
C(8)-H(8A)	0.9900	N(1B)-Fe(1)-P(3)	80.8(4)
C(8)-H(8B)	0.9900	P(2)-Fe(1)-P(3)	88.91(5)
C(9)-C(10)	1.527(7)	P(1)-Fe(1)-P(3)	90.62(5)
C(9)-H(9A)	0.9900	H(201)-Fe(1)-Fe(2)	28.2(10)
C(9)-H(9B)	0.9900	H(200)-Fe(1)-Fe(2)	28.2(10)
C(10)-C(11)	1.530(7)	N(1A)-Fe(1)-Fe(2)	42.14(18)
C(10)-H(10A)	0.9900	N(1B)-Fe(1)-Fe(2)	45.1(4)
C(10)-H(10B)	0.9900	P(2)-Fe(1)-Fe(2)	123.97(4)
C(11)-C(12)	1.468(6)	P(1)-Fe(1)-Fe(2)	127.28(4)
C(11)-H(11A)	0.9900	P(3)-Fe(1)-Fe(2)	125.50(4)
C(11)-H(11B)	0.9900	H(201)-Fe(1)-H(200)	54.0(19)
C(12)-H(12A)	0.9900	H(200)-Fe(1)-H(200)	0(4)
C(12)-H(12B)	0.9900	N(1A)-Fe(1)-H(200)	70.3(10)
C(13)-C(14)	1.497(6)	N(1B)-Fe(1)-H(200)	25(2)
C(13)-H(13A)	0.9900	P(2)-Fe(1)-H(200)	114(2)
C(13)-H(13B)	0.9900	P(1)-Fe(1)-H(200)	153.5(16)

P(3)-Fe(1)-H(200)	102.5(15)	Fe(1)-Fe(2)-H(201)	28.2(10)
Fe(2)-Fe(1)-H(200)	28.2(10)	H(200)-Fe(2)-H(201)	54.0(19)
H(201)-Fe(1)-H(201)	0(2)	Fe(2)-N(1A)-Fe(1)	94.7(3)
H(200)-Fe(1)-H(201)	54.0(19)	Fe(2)-N(1A)-H(1C)	132.7
N(1A)-Fe(1)-H(201)	24.6(3)	Fe(1)-N(1A)-H(1C)	132.7
N(1B)-Fe(1)-H(201)	73.3(11)	Fe(2)-N(1A)-H(201)	56.5(10)
P(2)-Fe(1)-H(201)	111.5(5)	Fe(1)-N(1A)-H(201)	54.1(9)
P(1)-Fe(1)-H(201)	106.4(8)	H(1C)-N(1A)-H(201)	147.1
P(3)-Fe(1)-H(201)	153.2(9)	Fe(1)-N(1B)-Fe(2)	90.3(7)
Fe(2)-Fe(1)-H(201)	28.2(10)	Fe(1)-N(1B)-H(200)	51.8(15)
H(200)-Fe(1)-H(201)	54.0(19)	Fe(2)-N(1B)-H(200)	50.8(17)
H(200)-Fe(2)-H(201)	54.0(19)	Fe(1)-N(1B)-H(1D)	134.8
H(200)-Fe(2)-N(1A)	71.3(10)	Fe(2)-N(1B)-H(1D)	134.8
H(201)-Fe(2)-N(1A)	25.3(4)	H(200)-N(1B)-H(1D)	152.4
H(200)-Fe(2)-N(1B)	25(2)	C(21)-P(1)-C(39)	105.94(19)
H(201)-Fe(2)-N(1B)	72.8(10)	C(21)-P(1)-C(33)	99.41(18)
N(1A)-Fe(2)-N(1B)	82.5(4)	C(39)-P(1)-C(33)	96.55(19)
H(200)-Fe(2)-P(4)	106(2)	C(21)-P(1)-Fe(1)	118.31(13)
H(201)-Fe(2)-P(4)	118.1(3)	C(39)-P(1)-Fe(1)	111.94(14)
N(1A)-Fe(2)-P(4)	136.4(2)	C(33)-P(1)-Fe(1)	121.58(14)
N(1B)-Fe(2)-P(4)	113.91(15)	C(23)-P(2)-C(57)	105.29(18)
H(200)-Fe(2)-P(5)	105.8(18)	C(23)-P(2)-C(63)	99.87(18)
H(201)-Fe(2)-P(5)	150.0(8)	C(57)-P(2)-C(63)	96.46(18)
N(1A)-Fe(2)-P(5)	136.2(2)	C(23)-P(2)-Fe(1)	116.10(13)
N(1B)-Fe(2)-P(5)	82.6(4)	C(57)-P(2)-Fe(1)	112.14(13)
P(4)-Fe(2)-P(5)	87.18(5)	C(63)-P(2)-Fe(1)	123.95(14)
H(200)-Fe(2)-P(6)	158.9(10)	C(22)-P(3)-C(51)	101.22(18)
H(201)-Fe(2)-P(6)	106.1(9)	C(22)-P(3)-C(45)	103.17(19)
N(1A)-Fe(2)-P(6)	87.58(18)	C(51)-P(3)-C(45)	96.87(19)
N(1B)-Fe(2)-P(6)	155.21(4)	C(22)-P(3)-Fe(1)	115.74(13)
P(4)-Fe(2)-P(6)	88.83(5)	C(51)-P(3)-Fe(1)	118.00(15)
P(5)-Fe(2)-P(6)	89.07(5)	C(45)-P(3)-Fe(1)	118.68(13)
H(200)-Fe(2)-Fe(1)	28.2(10)	C(24)-P(4)-C(75)	104.46(18)
H(201)-Fe(2)-Fe(1)	28.2(10)	C(24)-P(4)-C(69)	102.74(18)
N(1A)-Fe(2)-Fe(1)	43.17(18)	C(75)-P(4)-C(69)	96.58(18)
N(1B)-Fe(2)-Fe(1)	44.6(4)	C(24)-P(4)-Fe(2)	114.13(13)
P(4)-Fe(2)-Fe(1)	123.17(4)	C(75)-P(4)-Fe(2)	114.94(14)
P(5)-Fe(2)-Fe(1)	125.01(4)	C(69)-P(4)-Fe(2)	121.35(13)
P(6)-Fe(2)-Fe(1)	130.72(4)	C(25)-P(5)-C(81)	103.19(18)
H(200)-Fe(2)-H(200)	0.00(13)	C(25)-P(5)-C(87)	104.23(19)
H(201)-Fe(2)-H(200)	54.0(19)	C(81)-P(5)-C(87)	95.83(18)
N(1A)-Fe(2)-H(200)	71.3(10)	C(25)-P(5)-Fe(2)	115.93(13)
N(1B)-Fe(2)-H(200)	25(2)	C(81)-P(5)-Fe(2)	122.19(13)
P(4)-Fe(2)-H(200)	106(2)	C(87)-P(5)-Fe(2)	112.42(15)
P(5)-Fe(2)-H(200)	105.8(18)	C(26)-P(6)-C(99)	104.14(19)
P(6)-Fe(2)-H(200)	158.9(10)	C(26)-P(6)-C(93)	105.40(18)
Fe(1)-Fe(2)-H(200)	28.2(10)	C(99)-P(6)-C(93)	96.12(18)
H(200)-Fe(2)-H(201)	54.0(19)	C(26)-P(6)-Fe(2)	114.78(14)
H(201)-Fe(2)-H(201)	0.0(16)	C(99)-P(6)-Fe(2)	114.64(14)
N(1A)-Fe(2)-H(201)	25.3(4)	C(93)-P(6)-Fe(2)	119.26(13)
N(1B)-Fe(2)-H(201)	72.8(10)	C(23)-B(1)-C(27)	110.8(3)
P(4)-Fe(2)-H(201)	118.1(3)	C(23)-B(1)-C(21)	109.8(3)
P(5)-Fe(2)-H(201)	150.0(8)	C(27)-B(1)-C(21)	108.9(3)
P(6)-Fe(2)-H(201)	106.1(9)	C(23)-B(1)-C(22)	110.7(3)

C(27)-B(1)-C(22)	107.3(3)	C(31)-C(30)-H(30)	120.1
C(21)-B(1)-C(22)	109.3(3)	C(29)-C(30)-H(30)	120.1
C(25)-B(2)-C(110)	109.6(3)	C(30)-C(31)-C(32)	120.8(5)
C(25)-B(2)-C(26)	108.9(3)	C(30)-C(31)-H(31)	119.6
C(110)-B(2)-C(26)	112.1(3)	C(32)-C(31)-H(31)	119.6
C(25)-B(2)-C(24)	109.7(3)	C(31)-C(32)-C(27)	122.0(4)
C(110)-B(2)-C(24)	106.5(3)	C(31)-C(32)-H(32)	119.0
C(26)-B(2)-C(24)	109.9(3)	C(27)-C(32)-H(32)	119.0
B(1)-C(21)-P(1)	113.9(3)	C(34)-C(33)-C(38)	117.2(4)
B(1)-C(21)-H(21A)	108.8	C(34)-C(33)-P(1)	122.9(3)
P(1)-C(21)-H(21A)	108.8	C(38)-C(33)-P(1)	119.8(3)
B(1)-C(21)-H(21B)	108.8	C(33)-C(34)-C(35)	121.0(4)
P(1)-C(21)-H(21B)	108.8	C(33)-C(34)-H(34)	119.5
H(21A)-C(21)-H(21B)	107.7	C(35)-C(34)-H(34)	119.5
B(1)-C(22)-P(3)	115.3(3)	C(36)-C(35)-C(34)	120.6(4)
B(1)-C(22)-H(22A)	108.4	C(36)-C(35)-H(35)	119.7
P(3)-C(22)-H(22A)	108.4	C(34)-C(35)-H(35)	119.7
B(1)-C(22)-H(22B)	108.4	C(35)-C(36)-C(37)	119.0(4)
P(3)-C(22)-H(22B)	108.4	C(35)-C(36)-H(36)	120.5
H(22A)-C(22)-H(22B)	107.5	C(37)-C(36)-H(36)	120.5
B(1)-C(23)-P(2)	116.7(3)	C(36)-C(37)-C(38)	121.4(4)
B(1)-C(23)-H(23A)	108.1	C(36)-C(37)-H(37)	119.3
P(2)-C(23)-H(23A)	108.1	C(38)-C(37)-H(37)	119.3
B(1)-C(23)-H(23B)	108.1	C(37)-C(38)-C(33)	120.7(4)
P(2)-C(23)-H(23B)	108.1	C(37)-C(38)-H(38)	119.6
H(23A)-C(23)-H(23B)	107.3	C(33)-C(38)-H(38)	119.6
B(2)-C(24)-P(4)	113.6(3)	C(40)-C(39)-C(44)	117.1(4)
B(2)-C(24)-H(24A)	108.9	C(40)-C(39)-P(1)	125.0(3)
P(4)-C(24)-H(24A)	108.9	C(44)-C(39)-P(1)	117.9(3)
B(2)-C(24)-H(24B)	108.9	C(39)-C(40)-C(41)	121.3(4)
P(4)-C(24)-H(24B)	108.9	C(39)-C(40)-H(40)	119.3
H(24A)-C(24)-H(24B)	107.7	C(41)-C(40)-H(40)	119.3
B(2)-C(25)-P(5)	113.8(3)	C(42)-C(41)-C(40)	119.5(4)
B(2)-C(25)-H(25A)	108.8	C(42)-C(41)-H(41)	120.2
P(5)-C(25)-H(25A)	108.8	C(40)-C(41)-H(41)	120.2
B(2)-C(25)-H(25B)	108.8	C(41)-C(42)-C(43)	120.8(4)
P(5)-C(25)-H(25B)	108.8	C(41)-C(42)-H(42)	119.6
H(25A)-C(25)-H(25B)	107.7	C(43)-C(42)-H(42)	119.6
B(2)-C(26)-P(6)	113.3(3)	C(42)-C(43)-C(44)	118.6(4)
B(2)-C(26)-H(26A)	108.9	C(42)-C(43)-H(43)	120.7
P(6)-C(26)-H(26A)	108.9	C(44)-C(43)-H(43)	120.7
B(2)-C(26)-H(26B)	108.9	C(39)-C(44)-C(43)	122.6(4)
P(6)-C(26)-H(26B)	108.9	C(39)-C(44)-H(44)	118.7
H(26A)-C(26)-H(26B)	107.7	C(43)-C(44)-H(44)	118.7
C(28)-C(27)-C(32)	114.7(4)	C(50)-C(45)-C(46)	117.8(4)
C(28)-C(27)-B(1)	124.2(4)	C(50)-C(45)-P(3)	119.4(3)
C(32)-C(27)-B(1)	121.1(4)	C(46)-C(45)-P(3)	122.8(3)
C(27)-C(28)-C(29)	124.8(4)	C(45)-C(46)-C(47)	120.4(4)
C(27)-C(28)-H(28)	117.6	C(45)-C(46)-H(46)	119.8
C(29)-C(28)-H(28)	117.6	C(47)-C(46)-H(46)	119.8
C(30)-C(29)-C(28)	117.9(4)	C(48)-C(47)-C(46)	119.8(4)
C(30)-C(29)-H(29)	121.1	C(48)-C(47)-H(47)	120.1
C(28)-C(29)-H(29)	121.1	C(46)-C(47)-H(47)	120.1
C(31)-C(30)-C(29)	119.8(4)	C(47)-C(48)-C(49)	120.3(4)

C(47)-C(48)-H(48)	119.9	C(67)-C(66)-H(66)	120.5
C(49)-C(48)-H(48)	119.9	C(65)-C(66)-H(66)	120.5
C(50)-C(49)-C(48)	120.3(5)	C(66)-C(67)-C(68)	120.1(4)
C(50)-C(49)-H(49)	119.9	C(66)-C(67)-H(67)	119.9
C(48)-C(49)-H(49)	119.9	C(68)-C(67)-H(67)	119.9
C(49)-C(50)-C(45)	121.4(4)	C(63)-C(68)-C(67)	121.3(4)
C(49)-C(50)-H(50)	119.3	C(63)-C(68)-H(68)	119.4
C(45)-C(50)-H(50)	119.3	C(67)-C(68)-H(68)	119.4
C(52)-C(51)-C(56)	118.0(4)	C(70)-C(69)-C(74)	117.6(4)
C(52)-C(51)-P(3)	120.7(3)	C(70)-C(69)-P(4)	121.4(3)
C(56)-C(51)-P(3)	121.2(3)	C(74)-C(69)-P(4)	120.9(3)
C(51)-C(52)-C(53)	120.6(4)	C(69)-C(70)-C(71)	121.6(4)
C(51)-C(52)-H(52)	119.7	C(69)-C(70)-H(70)	119.2
C(53)-C(52)-H(52)	119.7	C(71)-C(70)-H(70)	119.2
C(54)-C(53)-C(52)	120.9(4)	C(72)-C(71)-C(70)	119.8(4)
C(54)-C(53)-H(53)	119.5	C(72)-C(71)-H(71)	120.1
C(52)-C(53)-H(53)	119.5	C(70)-C(71)-H(71)	120.1
C(55)-C(54)-C(53)	119.4(4)	C(71)-C(72)-C(73)	119.4(4)
C(55)-C(54)-H(54)	120.3	C(71)-C(72)-H(72)	120.3
C(53)-C(54)-H(54)	120.3	C(73)-C(72)-H(72)	120.3
C(54)-C(55)-C(56)	119.9(4)	C(74)-C(73)-C(72)	119.9(4)
C(54)-C(55)-H(55)	120.1	C(74)-C(73)-H(73)	120.0
C(56)-C(55)-H(55)	120.1	C(72)-C(73)-H(73)	120.0
C(55)-C(56)-C(51)	121.2(4)	C(73)-C(74)-C(69)	121.7(4)
C(55)-C(56)-H(56)	119.4	C(73)-C(74)-H(74)	119.2
C(51)-C(56)-H(56)	119.4	C(69)-C(74)-H(74)	119.2
C(58)-C(57)-C(62)	117.5(4)	C(80)-C(75)-C(76)	118.1(4)
C(58)-C(57)-P(2)	124.9(3)	C(80)-C(75)-P(4)	118.2(3)
C(62)-C(57)-P(2)	117.5(3)	C(76)-C(75)-P(4)	123.5(3)
C(57)-C(58)-C(59)	120.9(4)	C(75)-C(76)-C(77)	120.8(4)
C(57)-C(58)-H(58)	119.6	C(75)-C(76)-H(76)	119.6
C(59)-C(58)-H(58)	119.6	C(77)-C(76)-H(76)	119.6
C(60)-C(59)-C(58)	120.1(4)	C(78)-C(77)-C(76)	119.8(4)
C(60)-C(59)-H(59)	120.0	C(78)-C(77)-H(77)	120.1
C(58)-C(59)-H(59)	120.0	C(76)-C(77)-H(77)	120.1
C(59)-C(60)-C(61)	119.8(4)	C(79)-C(78)-C(77)	120.2(4)
C(59)-C(60)-H(60)	120.1	C(79)-C(78)-H(78)	119.9
C(61)-C(60)-H(60)	120.1	C(77)-C(78)-H(78)	119.9
C(60)-C(61)-C(62)	120.4(4)	C(78)-C(79)-C(80)	119.9(4)
C(60)-C(61)-H(61)	119.8	C(78)-C(79)-H(79)	120.1
C(62)-C(61)-H(61)	119.8	C(80)-C(79)-H(79)	120.1
C(61)-C(62)-C(57)	121.4(4)	C(75)-C(80)-C(79)	121.2(4)
C(61)-C(62)-H(62)	119.3	C(75)-C(80)-H(80)	119.4
C(57)-C(62)-H(62)	119.3	C(79)-C(80)-H(80)	119.4
C(68)-C(63)-C(64)	118.3(4)	C(82)-C(81)-C(86)	116.5(4)
C(68)-C(63)-P(2)	121.6(3)	C(82)-C(81)-P(5)	122.7(3)
C(64)-C(63)-P(2)	119.9(3)	C(86)-C(81)-P(5)	120.9(3)
C(65)-C(64)-C(63)	120.4(4)	C(83)-C(82)-C(81)	121.5(4)
C(65)-C(64)-H(64)	119.8	C(83)-C(82)-H(82)	119.3
C(63)-C(64)-H(64)	119.8	C(81)-C(82)-H(82)	119.3
C(64)-C(65)-C(66)	120.9(4)	C(84)-C(83)-C(82)	121.2(4)
C(64)-C(65)-H(65)	119.5	C(84)-C(83)-H(83)	119.4
C(66)-C(65)-H(65)	119.5	C(82)-C(83)-H(83)	119.4
C(67)-C(66)-C(65)	119.0(4)	C(83)-C(84)-C(85)	119.1(4)

C(83)-C(84)-H(84)	120.4	C(103)-C(102)-H(102)	120.0
C(85)-C(84)-H(84)	120.4	C(101)-C(102)-H(102)	120.0
C(84)-C(85)-C(86)	119.5(4)	C(102)-C(103)-C(104)	119.9(4)
C(84)-C(85)-H(85)	120.3	C(102)-C(103)-H(103)	120.1
C(86)-C(85)-H(85)	120.3	C(104)-C(103)-H(103)	120.1
C(85)-C(86)-C(81)	122.2(4)	C(99)-C(104)-C(103)	121.3(4)
C(85)-C(86)-H(86)	118.9	C(99)-C(104)-H(104)	119.4
C(81)-C(86)-H(86)	118.9	C(103)-C(104)-H(104)	119.4
C(92)-C(87)-C(88)	118.4(4)	C(110)-C(105)-C(106)	122.6(4)
C(92)-C(87)-P(5)	119.9(3)	C(110)-C(105)-H(105)	118.7
C(88)-C(87)-P(5)	121.3(4)	C(106)-C(105)-H(105)	118.7
C(89)-C(88)-C(87)	120.9(5)	C(107)-C(106)-C(105)	121.1(4)
C(89)-C(88)-H(88)	119.6	C(107)-C(106)-H(106)	119.4
C(87)-C(88)-H(88)	119.6	C(105)-C(106)-H(106)	119.4
C(88)-C(89)-C(90)	118.8(5)	C(108)-C(107)-C(106)	117.9(4)
C(88)-C(89)-H(89)	120.6	C(108)-C(107)-H(107)	121.0
C(90)-C(89)-H(89)	120.6	C(106)-C(107)-H(107)	121.0
C(91)-C(90)-C(89)	121.3(4)	C(107)-C(108)-C(109)	121.3(4)
C(91)-C(90)-H(90)	119.4	C(107)-C(108)-H(108)	119.3
C(89)-C(90)-H(90)	119.4	C(109)-C(108)-H(108)	119.3
C(90)-C(91)-C(92)	119.7(4)	C(108)-C(109)-C(110)	122.1(4)
C(90)-C(91)-H(91)	120.2	C(108)-C(109)-H(109)	118.9
C(92)-C(91)-H(91)	120.2	C(110)-C(109)-H(109)	118.9
C(87)-C(92)-C(91)	121.0(4)	C(105)-C(110)-C(109)	114.9(4)
C(87)-C(92)-H(92)	119.5	C(105)-C(110)-B(2)	125.5(4)
C(91)-C(92)-H(92)	119.5	C(109)-C(110)-B(2)	119.6(4)
C(98)-C(93)-C(94)	118.2(4)	O(5)-Na(1)-O(4)	97.22(12)
C(98)-C(93)-P(6)	121.5(3)	O(5)-Na(1)-O(1)	97.40(14)
C(94)-C(93)-P(6)	120.2(3)	O(4)-Na(1)-O(1)	84.48(12)
C(95)-C(94)-C(93)	119.9(4)	O(5)-Na(1)-O(2)	92.57(12)
C(95)-C(94)-H(94)	120.1	O(4)-Na(1)-O(2)	169.12(15)
C(93)-C(94)-H(94)	120.1	O(1)-Na(1)-O(2)	89.59(14)
C(96)-C(95)-C(94)	121.0(4)	O(5)-Na(1)-O(3)	100.81(13)
C(96)-C(95)-H(95)	119.5	O(4)-Na(1)-O(3)	84.13(13)
C(94)-C(95)-H(95)	119.5	O(1)-Na(1)-O(3)	159.57(15)
C(95)-C(96)-C(97)	118.7(4)	O(2)-Na(1)-O(3)	98.72(14)
C(95)-C(96)-H(96)	120.6	C(4)-O(1)-C(1)	109.9(4)
C(97)-C(96)-H(96)	120.6	C(4)-O(1)-Na(1)	123.3(3)
C(96)-C(97)-C(98)	120.2(4)	C(1)-O(1)-Na(1)	121.9(3)
C(96)-C(97)-H(97)	119.9	C(5)-O(2)-C(8)	104.2(4)
C(98)-C(97)-H(97)	119.9	C(5)-O(2)-Na(1)	120.8(3)
C(93)-C(98)-C(97)	122.0(4)	C(8)-O(2)-Na(1)	134.9(3)
C(93)-C(98)-H(98)	119.0	C(13)-O(3)-C(16)	107.6(4)
C(97)-C(98)-H(98)	119.0	C(13)-O(3)-Na(1)	122.5(3)
C(104)-C(99)-C(100)	118.1(4)	C(16)-O(3)-Na(1)	129.3(3)
C(104)-C(99)-P(6)	118.9(3)	C(17)-O(4)-C(20)	106.8(3)
C(100)-C(99)-P(6)	122.9(3)	C(17)-O(4)-Na(1)	116.5(3)
C(101)-C(100)-C(99)	120.3(4)	C(20)-O(4)-Na(1)	136.6(3)
C(101)-C(100)-H(100)	119.9	C(12)-O(5)-C(9)	107.8(4)
C(99)-C(100)-H(100)	119.9	C(12)-O(5)-Na(1)	113.5(3)
C(102)-C(101)-C(100)	120.3(4)	C(9)-O(5)-Na(1)	123.5(3)
C(102)-C(101)-H(101)	119.8	O(1)-C(1)-C(2)	105.1(4)
C(100)-C(101)-H(101)	119.8	O(1)-C(1)-H(1A)	110.7
C(103)-C(102)-C(101)	120.0(4)	C(2)-C(1)-H(1A)	110.7

O(1)-C(1)-H(1B)	110.7	C(11)-C(10)-H(10B)	110.9
C(2)-C(1)-H(1B)	110.7	C(9)-C(10)-H(10B)	110.9
H(1A)-C(1)-H(1B)	108.8	H(10A)-C(10)-H(10B)	108.9
C(1)-C(2)-C(3)	103.2(5)	C(12)-C(11)-C(10)	103.3(5)
C(1)-C(2)-H(2A)	111.1	C(12)-C(11)-H(11A)	111.1
C(3)-C(2)-H(2A)	111.1	C(10)-C(11)-H(11A)	111.1
C(1)-C(2)-H(2B)	111.1	C(12)-C(11)-H(11B)	111.1
C(3)-C(2)-H(2B)	111.1	C(10)-C(11)-H(11B)	111.1
H(2A)-C(2)-H(2B)	109.1	H(11A)-C(11)-H(11B)	109.1
C(2)-C(3)-C(4)	103.5(4)	O(5)-C(12)-C(11)	104.2(4)
C(2)-C(3)-H(3A)	111.1	O(5)-C(12)-H(12A)	110.9
C(4)-C(3)-H(3A)	111.1	C(11)-C(12)-H(12A)	110.9
C(2)-C(3)-H(3B)	111.1	O(5)-C(12)-H(12B)	110.9
C(4)-C(3)-H(3B)	111.1	C(11)-C(12)-H(12B)	110.9
H(3A)-C(3)-H(3B)	109.0	H(12A)-C(12)-H(12B)	108.9
O(1)-C(4)-C(3)	105.7(4)	O(3)-C(13)-C(14)	103.7(4)
O(1)-C(4)-H(4A)	110.6	O(3)-C(13)-H(13A)	111.0
C(3)-C(4)-H(4A)	110.6	C(14)-C(13)-H(13A)	111.0
O(1)-C(4)-H(4B)	110.6	O(3)-C(13)-H(13B)	111.0
C(3)-C(4)-H(4B)	110.6	C(14)-C(13)-H(13B)	111.0
H(4A)-C(4)-H(4B)	108.7	H(13A)-C(13)-H(13B)	109.0
O(2)-C(5)-C(6)	107.3(5)	C(13)-C(14)-C(15)	102.8(4)
O(2)-C(5)-H(5A)	110.2	C(13)-C(14)-H(14A)	111.2
C(6)-C(5)-H(5A)	110.2	C(15)-C(14)-H(14A)	111.2
O(2)-C(5)-H(5B)	110.2	C(13)-C(14)-H(14B)	111.2
C(6)-C(5)-H(5B)	110.2	C(15)-C(14)-H(14B)	111.2
H(5A)-C(5)-H(5B)	108.5	H(14A)-C(14)-H(14B)	109.1
C(7)-C(6)-C(5)	103.7(6)	C(14)-C(15)-C(16)	102.7(4)
C(7)-C(6)-H(6A)	111.0	C(14)-C(15)-H(15A)	111.2
C(5)-C(6)-H(6A)	111.0	C(16)-C(15)-H(15A)	111.2
C(7)-C(6)-H(6B)	111.0	C(14)-C(15)-H(15B)	111.2
C(5)-C(6)-H(6B)	111.0	C(16)-C(15)-H(15B)	111.2
H(6A)-C(6)-H(6B)	109.0	H(15A)-C(15)-H(15B)	109.1
C(6)-C(7)-C(8)	104.9(5)	O(3)-C(16)-C(15)	106.9(4)
C(6)-C(7)-H(7A)	110.8	O(3)-C(16)-H(16A)	110.3
C(8)-C(7)-H(7A)	110.8	C(15)-C(16)-H(16A)	110.3
C(6)-C(7)-H(7B)	110.8	O(3)-C(16)-H(16B)	110.3
C(8)-C(7)-H(7B)	110.8	C(15)-C(16)-H(16B)	110.3
H(7A)-C(7)-H(7B)	108.8	H(16A)-C(16)-H(16B)	108.6
O(2)-C(8)-C(7)	105.5(5)	O(4)-C(17)-C(18)	107.0(4)
O(2)-C(8)-H(8A)	110.6	O(4)-C(17)-H(17A)	110.3
C(7)-C(8)-H(8A)	110.6	C(18)-C(17)-H(17A)	110.3
O(2)-C(8)-H(8B)	110.6	O(4)-C(17)-H(17B)	110.3
C(7)-C(8)-H(8B)	110.6	C(18)-C(17)-H(17B)	110.3
H(8A)-C(8)-H(8B)	108.8	H(17A)-C(17)-H(17B)	108.6
O(5)-C(9)-C(10)	105.6(4)	C(19)-C(18)-C(17)	105.3(4)
O(5)-C(9)-H(9A)	110.6	C(19)-C(18)-H(18A)	110.7
C(10)-C(9)-H(9A)	110.6	C(17)-C(18)-H(18A)	110.7
O(5)-C(9)-H(9B)	110.6	C(19)-C(18)-H(18B)	110.7
C(10)-C(9)-H(9B)	110.6	C(17)-C(18)-H(18B)	110.7
H(9A)-C(9)-H(9B)	108.8	H(18A)-C(18)-H(18B)	108.8
C(11)-C(10)-C(9)	104.3(4)	C(18)-C(19)-C(20)	103.0(4)
C(11)-C(10)-H(10A)	110.9	C(18)-C(19)-H(19A)	111.2
C(9)-C(10)-H(10A)	110.9	C(20)-C(19)-H(19A)	111.2

C(18)-C(19)-H(19B)	111.2
C(20)-C(19)-H(19B)	111.2
H(19A)-C(19)-H(19B)	109.1
O(4)-C(20)-C(19)	104.3(4)
O(4)-C(20)-H(20A)	110.9
C(19)-C(20)-H(20A)	110.9
O(4)-C(20)-H(20B)	110.9
C(19)-C(20)-H(20B)	110.9
H(20A)-C(20)-H(20B)	108.9

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [([$PhBP_3$]Fe)$_2$(μ-NH)(μ-H)][Na(THF)$_5$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2\ a^{*2} U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	241(4)	94(4)	132(3)	3(3)	-12(3)	25(3)
Fe(2)	220(4)	87(4)	123(3)	-7(3)	-2(3)	-12(3)
N(1A)	580(50)	650(50)	230(40)	40(30)	-10(30)	-450(40)
N(1B)	110(90)	460(100)	230(80)	-20(70)	-140(60)	-50(80)
P(1)	124(7)	112(7)	182(7)	12(5)	39(5)	17(5)
P(2)	147(7)	97(7)	160(6)	6(5)	15(5)	7(5)
P(3)	124(7)	109(7)	237(7)	20(6)	-10(5)	-11(5)
P(4)	135(7)	109(7)	152(6)	-8(5)	6(5)	-5(5)
P(5)	169(7)	100(7)	180(7)	-10(5)	32(5)	1(5)
P(6)	149(7)	87(7)	215(7)	6(6)	28(5)	2(5)
B(1)	210(30)	190(30)	50(30)	0(20)	-20(20)	30(20)
B(2)	170(30)	150(30)	100(30)	-60(20)	10(20)	-20(20)
C(21)	190(30)	130(30)	120(20)	-20(20)	-30(20)	0(20)
C(22)	130(30)	120(30)	160(20)	-20(20)	68(19)	0(20)
C(23)	110(30)	170(30)	100(20)	50(20)	19(19)	30(20)
C(24)	120(30)	190(30)	140(20)	-60(20)	-40(19)	-30(20)
C(25)	180(30)	120(20)	150(20)	30(20)	-64(19)	10(20)
C(26)	190(30)	130(20)	130(20)	30(20)	36(19)	60(20)
C(27)	150(30)	270(30)	150(20)	-20(20)	20(20)	-10(20)
C(28)	240(30)	170(30)	130(30)	-10(20)	0(20)	0(20)
C(29)	300(30)	370(30)	150(30)	50(30)	60(20)	30(30)
C(30)	370(30)	460(40)	160(30)	30(30)	40(20)	110(30)
C(31)	570(40)	290(30)	280(30)	-90(30)	30(30)	100(30)
C(32)	460(40)	230(30)	190(30)	-50(20)	30(20)	70(30)
C(33)	80(30)	140(30)	180(20)	50(20)	40(20)	-30(20)
C(34)	180(30)	140(30)	250(30)	50(20)	90(20)	-10(20)
C(35)	160(30)	150(30)	320(30)	10(20)	110(20)	110(20)
C(36)	70(30)	300(30)	390(30)	20(30)	10(20)	20(20)
C(37)	180(30)	240(30)	300(30)	-50(20)	10(20)	10(20)
C(38)	160(30)	210(30)	310(30)	-130(20)	50(20)	0(20)
C(39)	130(30)	120(30)	200(30)	-30(20)	20(20)	-30(20)
C(40)	180(30)	220(30)	180(30)	10(20)	0(20)	-10(20)
C(41)	230(30)	110(30)	370(30)	-80(20)	40(20)	10(20)
C(42)	170(30)	140(30)	530(40)	110(30)	10(30)	-50(20)
C(43)	240(30)	250(30)	420(30)	160(30)	150(20)	40(20)
C(44)	250(30)	180(30)	430(30)	70(30)	110(20)	90(20)
C(45)	100(30)	130(30)	200(30)	-30(20)	0(20)	40(20)
C(46)	190(30)	210(30)	270(30)	20(20)	50(20)	40(20)
C(47)	260(30)	140(30)	460(30)	-50(30)	200(30)	-70(20)
C(48)	170(30)	130(30)	600(40)	-130(30)	60(30)	-40(20)
C(49)	160(30)	130(30)	560(40)	-40(30)	-110(30)	30(20)
C(50)	130(30)	90(30)	440(30)	40(20)	-30(20)	-20(20)
C(51)	170(30)	100(30)	230(30)	-20(20)	-30(20)	20(20)
C(52)	190(30)	140(30)	460(30)	80(20)	80(20)	-40(20)
C(53)	160(30)	220(30)	500(30)	-40(30)	90(20)	70(20)
C(54)	250(30)	140(30)	420(30)	-40(30)	-10(30)	-10(20)
C(55)	310(30)	140(30)	260(30)	20(20)	-10(20)	10(20)
C(56)	170(30)	240(30)	250(30)	-130(20)	-30(20)	0(20)
C(57)	160(30)	60(20)	180(30)	0(20)	10(20)	-20(20)

C(58)	230(30)	160(30)	220(30)	10(20)	30(20)	-20(20)
C(59)	160(30)	250(30)	290(30)	0(20)	-20(20)	40(20)
C(60)	160(30)	70(30)	430(30)	-30(20)	70(30)	50(20)
C(61)	200(30)	100(30)	230(30)	-60(20)	60(20)	-10(20)
C(62)	180(30)	120(30)	190(30)	20(20)	-20(20)	10(20)
C(63)	140(30)	140(30)	90(20)	10(20)	30(20)	30(20)
C(64)	150(30)	160(30)	310(30)	10(20)	30(20)	0(20)
C(65)	250(30)	40(30)	360(30)	0(20)	0(20)	50(20)
C(66)	320(30)	40(30)	320(30)	0(20)	140(20)	-90(20)
C(67)	230(30)	200(30)	350(30)	-10(30)	30(20)	-40(30)
C(68)	180(30)	110(30)	230(30)	-40(20)	40(20)	20(20)
C(69)	120(30)	150(30)	100(20)	20(20)	1(19)	20(20)
C(70)	220(30)	130(30)	230(30)	0(20)	-40(20)	-20(20)
C(71)	210(30)	200(30)	240(30)	-30(20)	10(20)	40(20)
C(72)	290(30)	70(30)	260(30)	-20(20)	-90(20)	50(20)
C(73)	350(30)	50(30)	190(30)	40(20)	20(20)	-30(20)
C(74)	180(30)	140(30)	210(30)	-50(20)	10(20)	20(20)
C(75)	150(30)	90(30)	160(30)	-10(20)	-40(20)	20(20)
C(76)	230(30)	180(30)	230(30)	40(20)	10(20)	-30(20)
C(77)	290(30)	170(30)	210(30)	0(20)	-40(20)	-90(20)
C(78)	90(30)	200(30)	390(30)	40(30)	10(20)	-10(20)
C(79)	220(30)	220(30)	230(30)	0(20)	50(20)	0(20)
C(80)	200(30)	150(30)	240(30)	10(20)	-20(20)	-80(20)
C(81)	140(30)	100(30)	160(20)	0(20)	-30(20)	0(20)
C(82)	260(30)	140(30)	250(30)	10(20)	40(20)	30(20)
C(83)	120(30)	320(30)	350(30)	-10(30)	30(20)	-40(20)
C(84)	100(30)	310(30)	290(30)	40(20)	40(20)	-60(20)
C(85)	200(30)	170(30)	300(30)	10(20)	90(20)	110(20)
C(86)	200(30)	200(30)	200(30)	-10(20)	-10(20)	-40(20)
C(87)	190(30)	160(30)	180(30)	10(20)	50(20)	60(20)
C(88)	390(30)	140(30)	420(30)	-10(30)	-10(30)	30(30)
C(89)	340(30)	170(30)	460(40)	90(30)	10(30)	70(30)
C(90)	360(30)	130(30)	340(30)	10(30)	160(30)	-30(30)
C(91)	270(30)	180(30)	330(30)	-90(30)	100(20)	-130(20)
C(92)	210(30)	200(30)	270(30)	-20(20)	70(20)	0(20)
C(93)	150(30)	120(30)	140(20)	-20(20)	30(20)	-10(20)
C(94)	170(30)	180(30)	260(30)	10(20)	70(20)	-20(20)
C(95)	250(30)	120(30)	430(30)	60(20)	130(30)	-10(20)
C(96)	260(30)	160(30)	370(30)	-60(30)	50(30)	-50(20)
C(97)	130(30)	270(30)	300(30)	-90(30)	60(20)	-30(20)
C(98)	240(30)	100(30)	320(30)	60(20)	70(20)	-20(20)
C(99)	126(13)	124(13)	148(13)	-2(9)	-1(9)	-17(9)
C(100)	170(30)	180(30)	210(30)	40(20)	40(20)	-20(20)
C(101)	240(30)	250(30)	240(30)	0(20)	100(20)	20(20)
C(102)	100(30)	140(30)	330(30)	-60(20)	20(20)	0(20)
C(103)	160(30)	170(30)	290(30)	10(20)	-80(20)	-20(20)
C(104)	180(30)	150(30)	230(30)	-110(20)	20(20)	-50(20)
C(105)	220(30)	200(30)	200(30)	-40(20)	0(20)	20(20)
C(106)	320(30)	270(30)	140(30)	40(20)	110(20)	50(30)
C(107)	300(30)	390(30)	80(20)	-50(20)	-20(20)	160(30)
C(108)	270(30)	270(30)	260(30)	-70(30)	-60(20)	30(20)
C(109)	270(30)	270(30)	170(30)	10(20)	0(20)	50(20)
C(110)	200(30)	80(30)	160(30)	-20(20)	-10(20)	70(20)
Na(1)	309(12)	264(12)	506(13)	95(10)	104(10)	3(10)

O(1)	370(20)	270(20)	900(30)	70(20)	160(20)	-52(18)
O(2)	560(30)	310(20)	460(20)	70(19)	-60(20)	97(19)
O(3)	330(20)	340(20)	620(30)	140(20)	28(18)	-45(19)
O(4)	340(20)	300(20)	360(20)	63(17)	116(17)	146(17)
O(5)	270(20)	290(20)	540(20)	28(18)	-18(18)	-33(17)
C(1)	740(50)	460(50)	1520(70)	-340(40)	700(50)	-350(40)
C(2)	430(40)	700(50)	420(40)	-10(30)	80(30)	-240(30)
C(3)	330(40)	350(30)	420(30)	110(30)	-30(30)	-10(30)
C(4)	430(40)	420(40)	450(30)	130(30)	-40(30)	-180(30)
C(5)	830(50)	460(40)	670(50)	-210(40)	-290(40)	150(40)
C(6)	660(60)	1040(60)	1180(60)	-300(50)	-220(40)	340(50)
C(7)	940(60)	550(50)	750(50)	10(40)	-50(40)	420(40)
C(8)	660(50)	340(40)	780(50)	50(30)	-130(40)	110(30)
C(9)	330(40)	430(40)	420(30)	20(30)	140(30)	-10(30)
C(10)	460(50)	1120(60)	1210(60)	-860(50)	90(40)	70(40)
C(11)	600(50)	540(50)	760(50)	-290(40)	40(40)	-180(30)
C(12)	310(40)	420(40)	530(40)	140(30)	-50(30)	-180(30)
C(13)	460(40)	340(40)	560(40)	190(30)	-20(30)	-130(30)
C(14)	540(40)	410(40)	450(40)	10(30)	20(30)	-140(30)
C(15)	420(40)	250(40)	1050(50)	120(30)	-110(30)	-120(30)
C(16)	450(40)	420(40)	880(50)	10(30)	40(30)	30(30)
C(17)	620(40)	310(30)	340(30)	90(30)	150(30)	70(30)
C(18)	430(40)	480(40)	660(40)	240(30)	-120(30)	-110(30)
C(19)	340(40)	330(40)	1020(50)	150(40)	80(40)	130(30)
C(20)	570(40)	460(40)	590(40)	-50(30)	290(30)	40(30)

Table 5. Crystal data and structure refinement for $([PhBP_3]Fe)_2(\mu\text{-}N)\cdot 2$ THF.

Identification code	sdb48	
Empirical formula	$C_{98}\ H_{98}\ B_2\ Fe_2\ N\ O_2\ P_6$	
Formula weight	1640.91	
Temperature	96(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 23.519(5) Å	α= 90°.
	b = 13.524(3) Å	β= 95.178(4)°.
	c = 25.937(6) Å	γ = 90°.
Volume	8216(3) $Å^3$	
Z	4	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.522 mm^{-1}	
F(000)	3444	
Crystal size	0.11 x 0.26 x 0.28 mm^3	
Theta range for data collection	1.23 to 28.63°.	
Index ranges	-31<=h<=31, -18<=k<=17, -34<=l<=34	
Reflections collected	122560	
Independent reflections	19794 [R(int) = 0.0844]	
Completeness to theta = 28.63°	93.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19794 / 0 / 1000	
Goodness-of-fit on F^2	1.611	
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.0726	
R indices (all data)	R1 = 0.0991, wR2 = 0.0785	
Largest diff. peak and hole	1.018 and -0.900 $e.Å^{-3}$	

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ([$PhBP_3$]Fe)$_2$(μ-N)·2 THF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	579(1)	1988(1)	2914(1)	13(1)
Fe(2)	-567(1)	1980(1)	2168(1)	14(1)
N(1)	-75(1)	2293(1)	2644(1)	18(1)
P(1)	1054(1)	3312(1)	3255(1)	13(1)
P(2)	1428(1)	1467(1)	2591(1)	13(1)
P(3)	771(1)	1193(1)	3699(1)	14(1)
P(4)	-1407(1)	1855(1)	2474(1)	14(1)
P(5)	-820(1)	868(1)	1491(1)	16(1)
P(6)	-892(1)	3296(1)	1717(1)	15(1)
B(1)	1950(1)	1877(2)	3642(1)	14(1)
B(2)	-1885(1)	2048(2)	1370(1)	15(1)
O(1)	6846(1)	1008(2)	4303(1)	77(1)
O(2)	8007(1)	9157(2)	10177(1)	102(1)
C(1)	6796(2)	478(2)	4767(1)	57(1)
C(2)	7388(1)	420(2)	5043(1)	43(1)
C(3)	7787(2)	734(3)	4634(2)	61(1)
C(4)	7405(2)	735(3)	4154(2)	73(1)
C(5)	7905(2)	8233(3)	9947(2)	87(2)
C(6)	7342(2)	8285(3)	9626(2)	90(2)
C(7)	7329(2)	9318(3)	9474(2)	105(2)
C(8)	7714(2)	9855(3)	9861(1)	68(1)
C(9)	2572(1)	1854(2)	3981(1)	12(1)
C(10)	3024(1)	1244(2)	3867(1)	17(1)
C(11)	3541(1)	1217(2)	4169(1)	19(1)
C(12)	3630(1)	1799(2)	4603(1)	20(1)
C(13)	3192(1)	2416(2)	4732(1)	19(1)
C(14)	2680(1)	2429(2)	4425(1)	16(1)
C(15)	1786(1)	3048(2)	3503(1)	14(1)
C(16)	1955(1)	1177(2)	3118(1)	14(1)
C(17)	1477(1)	1439(2)	4018(1)	15(1)
C(18)	738(1)	4004(2)	3769(1)	15(1)
C(19)	263(1)	4592(2)	3627(1)	20(1)
C(20)	56(1)	5248(2)	3970(1)	24(1)
C(21)	312(1)	5326(2)	4466(1)	26(1)
C(22)	762(1)	4717(2)	4622(1)	30(1)
C(23)	973(1)	4058(2)	4279(1)	22(1)
C(24)	1109(1)	4358(2)	2811(1)	14(1)
C(25)	825(1)	4353(2)	2325(1)	17(1)
C(26)	840(1)	5173(2)	2007(1)	24(1)
C(27)	1144(1)	6007(2)	2178(1)	23(1)
C(28)	1439(1)	6005(2)	2664(1)	26(1)
C(29)	1422(1)	5189(2)	2978(1)	22(1)
C(30)	1780(1)	2352(2)	2192(1)	13(1)
C(31)	2315(1)	2750(2)	2342(1)	16(1)
C(32)	2570(1)	3411(2)	2028(1)	20(1)
C(33)	2297(1)	3670(2)	1556(1)	26(1)
C(34)	1770(1)	3269(2)	1395(1)	26(1)
C(35)	1510(1)	2623(2)	1710(1)	21(1)
C(36)	1413(1)	365(2)	2185(1)	13(1)

C(37)	1821(1)	195(2)	1840(1)	20(1)
C(38)	1818(1)	-665(2)	1551(1)	23(1)
C(39)	1409(1)	-1380(2)	1611(1)	24(1)
C(40)	1010(1)	-1238(2)	1957(1)	26(1)
C(41)	1010(1)	-366(2)	2245(1)	18(1)
C(42)	706(1)	-155(2)	3638(1)	14(1)
C(43)	1161(1)	-808(2)	3719(1)	22(1)
C(44)	1075(1)	-1817(2)	3649(1)	29(1)
C(45)	542(1)	-2191(2)	3516(1)	27(1)
C(46)	82(1)	-1553(2)	3444(1)	26(1)
C(47)	166(1)	-540(2)	3495(1)	20(1)
C(48)	291(1)	1439(2)	4197(1)	15(1)
C(49)	-188(1)	2024(2)	4104(1)	25(1)
C(50)	-534(1)	2222(2)	4497(1)	38(1)
C(51)	-404(1)	1852(2)	4987(1)	33(1)
C(52)	75(1)	1266(2)	5085(1)	29(1)
C(53)	415(1)	1055(2)	4693(1)	22(1)
C(54)	-2509(1)	2106(2)	1043(1)	14(1)
C(55)	-2927(1)	1387(2)	1110(1)	20(1)
C(56)	-3471(1)	1425(2)	862(1)	22(1)
C(57)	-3632(1)	2193(2)	535(1)	23(1)
C(58)	-3235(1)	2913(2)	448(1)	21(1)
C(59)	-2686(1)	2860(2)	698(1)	18(1)
C(60)	-2010(1)	2001(2)	1987(1)	16(1)
C(61)	-1557(1)	1032(2)	1205(1)	16(1)
C(62)	-1496(1)	3024(2)	1252(1)	17(1)
C(63)	-1484(1)	642(2)	2778(1)	15(1)
C(64)	-1299(1)	509(2)	3297(1)	19(1)
C(65)	-1347(1)	-400(2)	3532(1)	23(1)
C(66)	-1575(1)	-1200(2)	3251(1)	22(1)
C(67)	-1752(1)	-1078(2)	2734(1)	24(1)
C(68)	-1711(1)	-165(2)	2497(1)	19(1)
C(69)	-1575(1)	2660(2)	3005(1)	15(1)
C(70)	-1170(1)	3285(2)	3256(1)	18(1)
C(71)	-1311(1)	3865(2)	3665(1)	25(1)
C(72)	-1852(1)	3832(2)	3828(1)	28(1)
C(73)	-2263(1)	3221(2)	3576(1)	25(1)
C(74)	-2124(1)	2633(2)	3170(1)	20(1)
C(75)	-757(1)	-470(2)	1599(1)	16(1)
C(76)	-987(1)	-1105(2)	1214(1)	27(1)
C(77)	-948(1)	-2122(2)	1278(1)	32(1)
C(78)	-674(1)	-2507(2)	1726(1)	30(1)
C(79)	-451(1)	-1882(2)	2112(1)	28(1)
C(80)	-494(1)	-861(2)	2052(1)	20(1)
C(81)	-348(1)	996(2)	971(1)	16(1)
C(82)	-514(1)	1338(2)	477(1)	23(1)
C(83)	-132(1)	1419(2)	105(1)	25(1)
C(84)	429(1)	1159(2)	220(1)	29(1)
C(85)	609(1)	818(2)	713(1)	29(1)
C(86)	224(1)	733(2)	1081(1)	23(1)
C(87)	-398(1)	3902(2)	1314(1)	16(1)
C(88)	-520(1)	4852(2)	1115(1)	21(1)
C(89)	-188(1)	5258(2)	759(1)	27(1)
C(90)	258(1)	4723(2)	585(1)	30(1)
C(91)	377(1)	3791(2)	772(1)	28(1)
C(92)	56(1)	3385(2)	1138(1)	20(1)

C(93)	-1106(1)	4339(2)	2103(1)	16(1)
C(94)	-1667(1)	4624(2)	2128(1)	21(1)
C(95)	-1799(1)	5417(2)	2429(1)	27(1)
C(96)	-1376(1)	5953(2)	2705(1)	26(1)
C(97)	-812(1)	5678(2)	2684(1)	23(1)
C(98)	-680(1)	4876(2)	2389(1)	18(1)

Table 7. Bond lengths [Å] and angles [°] for $([PhBP_3]Fe)_2(\mu\text{-}N)\cdot 2$ THF.

Fe(1)-N(1)	1.683(2)	C(20)-C(21)	1.374(4)
Fe(1)-P(1)	2.2491(8)	C(21)-C(22)	1.374(3)
Fe(1)-P(3)	2.3122(8)	C(22)-C(23)	1.381(3)
Fe(1)-P(2)	2.3398(8)	C(24)-C(25)	1.372(3)
Fe(2)-N(1)	1.668(2)	C(24)-C(29)	1.391(3)
Fe(2)-P(4)	2.2016(8)	C(25)-C(26)	1.384(3)
Fe(2)-P(6)	2.2275(8)	C(26)-C(27)	1.388(3)
Fe(2)-P(5)	2.3479(8)	C(27)-C(28)	1.381(3)
P(1)-C(15)	1.818(2)	C(28)-C(29)	1.374(3)
P(1)-C(24)	1.835(2)	C(30)-C(31)	1.390(3)
P(1)-C(18)	1.840(2)	C(30)-C(35)	1.401(3)
P(2)-C(16)	1.804(2)	C(31)-C(32)	1.385(3)
P(2)-C(36)	1.824(2)	C(32)-C(33)	1.375(3)
P(2)-C(30)	1.829(2)	C(33)-C(34)	1.384(3)
P(3)-C(17)	1.818(2)	C(34)-C(35)	1.375(3)
P(3)-C(48)	1.822(2)	C(36)-C(41)	1.387(3)
P(3)-C(42)	1.835(2)	C(36)-C(37)	1.391(3)
P(4)-C(60)	1.822(2)	C(37)-C(38)	1.383(3)
P(4)-C(69)	1.827(2)	C(38)-C(39)	1.382(3)
P(4)-C(63)	1.836(2)	C(39)-C(40)	1.370(3)
P(5)-C(81)	1.833(3)	C(40)-C(41)	1.395(3)
P(5)-C(75)	1.834(2)	C(42)-C(43)	1.388(3)
P(5)-C(61)	1.835(2)	C(42)-C(47)	1.392(3)
P(6)-C(62)	1.816(2)	C(43)-C(44)	1.389(3)
P(6)-C(87)	1.825(2)	C(44)-C(45)	1.366(4)
P(6)-C(93)	1.827(2)	C(45)-C(46)	1.383(4)
B(1)-C(9)	1.637(4)	C(46)-C(47)	1.388(3)
B(1)-C(17)	1.652(3)	C(48)-C(49)	1.380(3)
B(1)-C(16)	1.657(3)	C(48)-C(53)	1.392(3)
B(1)-C(15)	1.663(3)	C(49)-C(50)	1.385(3)
B(2)-C(54)	1.631(4)	C(50)-C(51)	1.375(4)
B(2)-C(62)	1.650(3)	C(51)-C(52)	1.382(4)
B(2)-C(61)	1.651(3)	C(52)-C(53)	1.379(3)
B(2)-C(60)	1.656(4)	C(54)-C(59)	1.395(3)
O(1)-C(1)	1.414(4)	C(54)-C(55)	1.404(3)
O(1)-C(4)	1.453(4)	C(55)-C(56)	1.381(3)
O(2)-C(8)	1.391(4)	C(56)-C(57)	1.372(3)
O(2)-C(5)	1.397(4)	C(57)-C(58)	1.380(3)
C(1)-C(2)	1.511(4)	C(58)-C(59)	1.393(3)
C(2)-C(3)	1.537(4)	C(63)-C(64)	1.387(3)
C(3)-C(4)	1.469(5)	C(63)-C(68)	1.391(3)
C(5)-C(6)	1.499(5)	C(64)-C(65)	1.381(3)
C(6)-C(7)	1.452(5)	C(65)-C(66)	1.386(3)
C(7)-C(8)	1.482(5)	C(66)-C(67)	1.376(3)
C(9)-C(14)	1.394(3)	C(67)-C(68)	1.387(3)
C(9)-C(10)	1.399(3)	C(69)-C(70)	1.390(3)
C(10)-C(11)	1.387(3)	C(69)-C(74)	1.396(3)
C(11)-C(12)	1.373(3)	C(70)-C(71)	1.384(3)
C(12)-C(13)	1.390(3)	C(71)-C(72)	1.377(4)
C(13)-C(14)	1.382(3)	C(72)-C(73)	1.389(3)
C(18)-C(23)	1.390(3)	C(73)-C(74)	1.381(3)
C(18)-C(19)	1.393(3)	C(75)-C(80)	1.383(3)
C(19)-C(20)	1.377(3)	C(75)-C(76)	1.390(3)

C(76)-C(77)	1.389(3)
C(77)-C(78)	1.377(4)
C(78)-C(79)	1.378(3)
C(79)-C(80)	1.392(3)
C(81)-C(82)	1.384(3)
C(81)-C(86)	1.397(3)
C(82)-C(83)	1.381(3)
C(83)-C(84)	1.373(4)
C(84)-C(85)	1.388(4)
C(85)-C(86)	1.379(3)
C(87)-C(92)	1.386(3)
C(87)-C(88)	1.404(3)
C(88)-C(89)	1.376(3)
C(89)-C(90)	1.383(4)
C(90)-C(91)	1.370(4)
C(91)-C(92)	1.381(3)
C(93)-C(94)	1.382(3)
C(93)-C(98)	1.396(3)
C(94)-C(95)	1.378(3)
C(95)-C(96)	1.378(4)
C(96)-C(97)	1.381(3)
C(97)-C(98)	1.379(3)

N(1)-Fe(1)-P(1)	111.76(7)
N(1)-Fe(1)-P(3)	125.35(7)
P(1)-Fe(1)-P(3)	88.45(3)
N(1)-Fe(1)-P(2)	134.60(7)
P(1)-Fe(1)-P(2)	88.37(3)
P(3)-Fe(1)-P(2)	94.03(3)
N(1)-Fe(2)-P(4)	109.78(7)
N(1)-Fe(2)-P(6)	111.64(7)
P(4)-Fe(2)-P(6)	88.56(3)
N(1)-Fe(2)-P(5)	145.89(7)
P(4)-Fe(2)-P(5)	92.52(3)
P(6)-Fe(2)-P(5)	93.84(3)
Fe(2)-N(1)-Fe(1)	142.41(12)
C(15)-P(1)-C(24)	104.75(11)
C(15)-P(1)-C(18)	105.96(11)
C(24)-P(1)-C(18)	96.81(11)
C(15)-P(1)-Fe(1)	113.79(8)
C(24)-P(1)-Fe(1)	115.31(8)
C(18)-P(1)-Fe(1)	118.16(8)
C(16)-P(2)-C(36)	103.66(11)
C(16)-P(2)-C(30)	104.76(11)
C(36)-P(2)-C(30)	101.20(11)
C(16)-P(2)-Fe(1)	110.17(8)
C(36)-P(2)-Fe(1)	118.64(8)
C(30)-P(2)-Fe(1)	116.76(8)
C(17)-P(3)-C(48)	104.12(11)
C(17)-P(3)-C(42)	106.73(11)
C(48)-P(3)-C(42)	101.04(11)
C(17)-P(3)-Fe(1)	114.37(8)
C(48)-P(3)-Fe(1)	117.10(9)
C(42)-P(3)-Fe(1)	112.14(8)
C(60)-P(4)-C(69)	104.43(11)
C(60)-P(4)-C(63)	107.11(11)
C(69)-P(4)-C(63)	99.91(11)
C(60)-P(4)-Fe(2)	114.19(8)
C(69)-P(4)-Fe(2)	119.20(8)
C(63)-P(4)-Fe(2)	110.52(8)
C(81)-P(5)-C(75)	99.16(11)
C(81)-P(5)-C(61)	107.63(11)
C(75)-P(5)-C(61)	103.99(11)
C(81)-P(5)-Fe(2)	111.12(8)
C(75)-P(5)-Fe(2)	120.42(9)
C(61)-P(5)-Fe(2)	113.08(8)
C(62)-P(6)-C(87)	102.20(11)
C(62)-P(6)-C(93)	106.37(12)
C(87)-P(6)-C(93)	100.89(11)
C(62)-P(6)-Fe(2)	113.44(8)
C(87)-P(6)-Fe(2)	117.00(8)
C(93)-P(6)-Fe(2)	115.29(8)
C(9)-B(1)-C(17)	107.05(19)
C(9)-B(1)-C(16)	110.92(19)
C(17)-B(1)-C(16)	109.51(19)
C(9)-B(1)-C(15)	108.27(19)
C(17)-B(1)-C(15)	108.31(19)
C(16)-B(1)-C(15)	112.59(19)
C(54)-B(2)-C(62)	110.7(2)
C(54)-B(2)-C(61)	109.0(2)
C(62)-B(2)-C(61)	109.75(19)
C(54)-B(2)-C(60)	105.93(19)
C(62)-B(2)-C(60)	111.1(2)
C(61)-B(2)-C(60)	110.3(2)
C(1)-O(1)-C(4)	104.1(3)
C(8)-O(2)-C(5)	107.4(3)
O(1)-C(1)-C(2)	106.7(3)
C(1)-C(2)-C(3)	104.5(3)
C(4)-C(3)-C(2)	102.9(3)
O(1)-C(4)-C(3)	105.8(3)
O(2)-C(5)-C(6)	107.7(3)
C(7)-C(6)-C(5)	101.1(3)
C(6)-C(7)-C(8)	106.9(3)
O(2)-C(8)-C(7)	107.8(3)
C(14)-C(9)-C(10)	114.7(2)
C(14)-C(9)-B(1)	121.4(2)
C(10)-C(9)-B(1)	123.9(2)
C(11)-C(10)-C(9)	122.8(2)
C(12)-C(11)-C(10)	120.5(2)
C(11)-C(12)-C(13)	118.8(2)
C(14)-C(13)-C(12)	119.6(2)
C(13)-C(14)-C(9)	123.6(2)
B(1)-C(15)-P(1)	117.24(16)
B(1)-C(16)-P(2)	116.23(16)
B(1)-C(17)-P(3)	115.72(16)
C(23)-C(18)-C(19)	117.6(2)
C(23)-C(18)-P(1)	124.41(19)
C(19)-C(18)-P(1)	117.71(19)
C(20)-C(19)-C(18)	121.2(2)
C(21)-C(20)-C(19)	120.3(3)
C(22)-C(21)-C(20)	119.4(2)
C(21)-C(22)-C(23)	120.6(3)

C(22)-C(23)-C(18)	120.8(2)
C(25)-C(24)-C(29)	119.3(2)
C(25)-C(24)-P(1)	121.05(19)
C(29)-C(24)-P(1)	119.53(19)
C(24)-C(25)-C(26)	120.5(2)
C(25)-C(26)-C(27)	120.1(3)
C(28)-C(27)-C(26)	119.4(2)
C(29)-C(28)-C(27)	120.3(2)
C(28)-C(29)-C(24)	120.4(2)
C(31)-C(30)-C(35)	118.3(2)
C(31)-C(30)-P(2)	122.66(18)
C(35)-C(30)-P(2)	119.00(18)
C(32)-C(31)-C(30)	121.0(2)
C(33)-C(32)-C(31)	119.8(2)
C(32)-C(33)-C(34)	120.2(2)
C(35)-C(34)-C(33)	120.3(2)
C(34)-C(35)-C(30)	120.5(2)
C(41)-C(36)-C(37)	118.2(2)
C(41)-C(36)-P(2)	119.74(19)
C(37)-C(36)-P(2)	121.87(18)
C(38)-C(37)-C(36)	121.1(2)
C(39)-C(38)-C(37)	119.9(2)
C(40)-C(39)-C(38)	120.0(2)
C(39)-C(40)-C(41)	120.1(2)
C(36)-C(41)-C(40)	120.7(2)
C(43)-C(42)-C(47)	118.3(2)
C(43)-C(42)-P(3)	124.16(19)
C(47)-C(42)-P(3)	117.50(18)
C(42)-C(43)-C(44)	120.3(2)
C(45)-C(44)-C(43)	121.0(3)
C(44)-C(45)-C(46)	119.5(2)
C(45)-C(46)-C(47)	120.0(2)
C(46)-C(47)-C(42)	120.8(2)
C(49)-C(48)-C(53)	118.3(2)
C(49)-C(48)-P(3)	122.0(2)
C(53)-C(48)-P(3)	119.6(2)
C(48)-C(49)-C(50)	120.4(3)
C(51)-C(50)-C(49)	120.9(3)
C(50)-C(51)-C(52)	119.1(3)
C(53)-C(52)-C(51)	120.1(3)
C(52)-C(53)-C(48)	121.1(3)
C(59)-C(54)-C(55)	114.5(2)
C(59)-C(54)-B(2)	124.8(2)
C(55)-C(54)-B(2)	120.6(2)
C(56)-C(55)-C(54)	123.0(2)
C(57)-C(56)-C(55)	120.5(2)
C(56)-C(57)-C(58)	118.8(2)
C(57)-C(58)-C(59)	120.0(2)
C(58)-C(59)-C(54)	123.1(2)
B(2)-C(60)-P(4)	118.61(16)
B(2)-C(61)-P(5)	116.22(16)
B(2)-C(62)-P(6)	116.94(17)
C(64)-C(63)-C(68)	118.5(2)
C(64)-C(63)-P(4)	119.86(19)
C(68)-C(63)-P(4)	121.58(19)
C(65)-C(64)-C(63)	120.9(2)
C(64)-C(65)-C(66)	120.3(2)
C(67)-C(66)-C(65)	119.2(2)
C(66)-C(67)-C(68)	120.7(2)
C(67)-C(68)-C(63)	120.4(2)
C(70)-C(69)-C(74)	119.1(2)
C(70)-C(69)-P(4)	121.93(19)
C(74)-C(69)-P(4)	119.00(19)
C(71)-C(70)-C(69)	120.1(2)
C(72)-C(71)-C(70)	120.7(3)
C(71)-C(72)-C(73)	119.7(3)
C(74)-C(73)-C(72)	120.0(3)
C(73)-C(74)-C(69)	120.5(2)
C(80)-C(75)-C(76)	119.4(2)
C(80)-C(75)-P(5)	122.03(19)
C(76)-C(75)-P(5)	118.60(19)
C(77)-C(76)-C(75)	120.5(3)
C(78)-C(77)-C(76)	119.8(3)
C(77)-C(78)-C(79)	120.0(2)
C(78)-C(79)-C(80)	120.5(3)
C(75)-C(80)-C(79)	119.8(2)
C(82)-C(81)-C(86)	117.5(2)
C(82)-C(81)-P(5)	125.0(2)
C(86)-C(81)-P(5)	117.55(19)
C(83)-C(82)-C(81)	121.7(3)
C(84)-C(83)-C(82)	120.0(3)
C(83)-C(84)-C(85)	119.6(3)
C(86)-C(85)-C(84)	120.0(3)
C(85)-C(86)-C(81)	121.2(2)
C(92)-C(87)-C(88)	118.7(2)
C(92)-C(87)-P(6)	120.64(19)
C(88)-C(87)-P(6)	120.06(19)
C(89)-C(88)-C(87)	120.1(3)
C(88)-C(89)-C(90)	120.2(3)
C(91)-C(90)-C(89)	120.2(3)
C(90)-C(91)-C(92)	120.2(3)
C(91)-C(92)-C(87)	120.7(2)
C(94)-C(93)-C(98)	118.2(2)
C(94)-C(93)-P(6)	123.6(2)
C(98)-C(93)-P(6)	118.22(19)
C(95)-C(94)-C(93)	120.5(3)
C(96)-C(95)-C(94)	121.0(3)
C(95)-C(96)-C(97)	119.3(2)
C(98)-C(97)-C(96)	119.9(3)
C(97)-C(98)-C(93)	121.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $([PhBP_3]Fe)_2(\mu\text{-}N)\cdot 2\ THF$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	11(1)	12(1)	14(1)	0(1)	1(1)	-1(1)
Fe(2)	12(1)	13(1)	17(1)	0(1)	1(1)	0(1)
N(1)	21(1)	13(1)	21(1)	-1(1)	7(1)	1(1)
P(1)	13(1)	13(1)	14(1)	0(1)	1(1)	0(1)
P(2)	13(1)	13(1)	14(1)	-1(1)	2(1)	-1(1)
P(3)	13(1)	15(1)	16(1)	0(1)	2(1)	-2(1)
P(4)	14(1)	14(1)	16(1)	1(1)	1(1)	-1(1)
P(5)	15(1)	15(1)	17(1)	0(1)	1(1)	2(1)
P(6)	14(1)	13(1)	17(1)	0(1)	2(1)	-1(1)
B(1)	13(2)	15(2)	13(2)	-1(1)	0(1)	1(1)
B(2)	13(2)	14(2)	17(2)	1(1)	3(1)	-1(1)
O(1)	84(2)	58(2)	81(2)	31(2)	-33(2)	-10(2)
O(2)	130(3)	55(2)	108(3)	1(2)	-50(2)	-5(2)
C(1)	65(3)	47(2)	56(3)	15(2)	-2(2)	8(2)
C(2)	56(2)	41(2)	33(2)	7(2)	4(2)	13(2)
C(3)	59(3)	45(2)	82(3)	-8(2)	17(2)	5(2)
C(4)	79(3)	56(3)	86(4)	12(2)	19(3)	-17(2)
C(5)	80(3)	44(3)	133(4)	-18(3)	-17(3)	-6(2)
C(6)	96(4)	52(3)	111(4)	0(3)	-47(3)	-10(2)
C(7)	94(4)	110(4)	101(4)	44(3)	-42(3)	-13(3)
C(8)	112(4)	44(2)	47(3)	14(2)	-2(2)	-4(2)
C(9)	15(1)	11(1)	11(1)	4(1)	5(1)	-4(1)
C(10)	19(2)	13(1)	18(2)	0(1)	-1(1)	1(1)
C(11)	17(2)	17(1)	22(2)	0(1)	2(1)	8(1)
C(12)	13(1)	24(2)	22(2)	4(1)	-4(1)	0(1)
C(13)	21(2)	21(1)	14(1)	-2(1)	-1(1)	-4(1)
C(14)	15(1)	17(1)	17(1)	1(1)	4(1)	2(1)
C(15)	9(1)	18(1)	16(1)	-3(1)	1(1)	-2(1)
C(16)	13(1)	13(1)	16(1)	3(1)	2(1)	0(1)
C(17)	13(1)	15(1)	16(1)	-1(1)	-1(1)	-1(1)
C(18)	15(1)	10(1)	21(2)	1(1)	6(1)	-3(1)
C(19)	18(2)	23(2)	21(2)	2(1)	2(1)	-1(1)
C(20)	22(2)	20(2)	33(2)	2(1)	9(1)	4(1)
C(21)	35(2)	19(2)	26(2)	1(1)	16(1)	6(1)
C(22)	37(2)	35(2)	16(2)	-3(1)	1(1)	7(1)
C(23)	25(2)	23(2)	18(2)	1(1)	4(1)	7(1)
C(24)	13(1)	13(1)	16(1)	0(1)	7(1)	2(1)
C(25)	18(2)	16(1)	19(2)	-1(1)	5(1)	-3(1)
C(26)	26(2)	26(2)	19(2)	3(1)	1(1)	-2(1)
C(27)	26(2)	16(1)	28(2)	5(1)	10(1)	1(1)
C(28)	30(2)	18(2)	30(2)	-4(1)	6(1)	-9(1)
C(29)	24(2)	20(2)	21(2)	3(1)	-1(1)	-8(1)
C(30)	13(1)	11(1)	15(1)	-1(1)	4(1)	3(1)
C(31)	15(1)	15(1)	17(1)	0(1)	2(1)	1(1)
C(32)	17(2)	17(1)	27(2)	-2(1)	6(1)	-3(1)
C(33)	23(2)	22(2)	34(2)	10(1)	13(1)	1(1)
C(34)	22(2)	37(2)	21(2)	12(1)	0(1)	2(1)
C(35)	14(2)	24(2)	24(2)	3(1)	0(1)	0(1)
C(36)	15(1)	14(1)	11(1)	1(1)	-2(1)	4(1)

C(37)	16(2)	19(1)	25(2)	-4(1)	2(1)	-2(1)
C(38)	25(2)	22(2)	23(2)	-4(1)	5(1)	8(1)
C(39)	32(2)	17(2)	22(2)	-8(1)	-4(1)	6(1)
C(40)	26(2)	16(1)	36(2)	-3(1)	4(1)	-3(1)
C(41)	18(2)	18(1)	17(2)	-1(1)	4(1)	3(1)
C(42)	17(2)	16(1)	10(1)	0(1)	3(1)	0(1)
C(43)	17(2)	20(2)	28(2)	3(1)	6(1)	-1(1)
C(44)	33(2)	18(2)	36(2)	5(1)	11(1)	8(1)
C(45)	42(2)	11(1)	30(2)	-2(1)	11(2)	-4(1)
C(46)	28(2)	26(2)	24(2)	-4(1)	5(1)	-11(1)
C(47)	18(2)	20(1)	21(2)	0(1)	4(1)	-2(1)
C(48)	15(1)	14(1)	17(2)	-4(1)	3(1)	-7(1)
C(49)	26(2)	28(2)	22(2)	4(1)	6(1)	3(1)
C(50)	37(2)	39(2)	42(2)	8(2)	21(2)	17(2)
C(51)	39(2)	32(2)	30(2)	-6(2)	20(2)	0(2)
C(52)	35(2)	34(2)	19(2)	1(1)	7(1)	-9(1)
C(53)	21(2)	26(2)	19(2)	2(1)	2(1)	-1(1)
C(54)	14(1)	14(1)	14(1)	-3(1)	5(1)	1(1)
C(55)	18(2)	18(1)	23(2)	2(1)	0(1)	-1(1)
C(56)	17(2)	21(2)	28(2)	0(1)	-1(1)	-7(1)
C(57)	15(2)	27(2)	24(2)	-3(1)	-6(1)	3(1)
C(58)	26(2)	20(1)	17(2)	1(1)	1(1)	3(1)
C(59)	17(2)	20(1)	16(1)	-1(1)	1(1)	-6(1)
C(60)	10(1)	14(1)	22(2)	2(1)	0(1)	-1(1)
C(61)	13(1)	20(1)	14(1)	1(1)	1(1)	-2(1)
C(62)	14(1)	18(1)	18(1)	0(1)	0(1)	2(1)
C(63)	9(1)	19(1)	19(2)	0(1)	6(1)	2(1)
C(64)	18(2)	18(1)	20(2)	0(1)	0(1)	-2(1)
C(65)	23(2)	26(2)	21(2)	4(1)	2(1)	3(1)
C(66)	20(2)	18(1)	28(2)	5(1)	9(1)	-1(1)
C(67)	24(2)	18(2)	33(2)	-2(1)	7(1)	-6(1)
C(68)	19(2)	19(1)	18(2)	1(1)	3(1)	-3(1)
C(69)	18(2)	14(1)	12(1)	5(1)	1(1)	1(1)
C(70)	21(2)	15(1)	19(2)	2(1)	3(1)	1(1)
C(71)	33(2)	17(1)	24(2)	-1(1)	1(1)	-5(1)
C(72)	41(2)	20(2)	22(2)	-3(1)	7(1)	4(1)
C(73)	24(2)	24(2)	29(2)	2(1)	9(1)	5(1)
C(74)	20(2)	18(1)	22(2)	3(1)	4(1)	1(1)
C(75)	15(1)	15(1)	18(2)	-1(1)	5(1)	2(1)
C(76)	36(2)	24(2)	19(2)	-2(1)	-3(1)	6(1)
C(77)	47(2)	18(2)	31(2)	-5(1)	-2(2)	1(1)
C(78)	42(2)	15(2)	32(2)	2(1)	5(2)	4(1)
C(79)	38(2)	23(2)	24(2)	8(1)	1(1)	4(1)
C(80)	18(2)	18(1)	24(2)	0(1)	-1(1)	2(1)
C(81)	19(2)	15(1)	15(1)	-3(1)	4(1)	0(1)
C(82)	20(2)	26(2)	23(2)	1(1)	2(1)	3(1)
C(83)	29(2)	28(2)	19(2)	2(1)	2(1)	-1(1)
C(84)	29(2)	32(2)	29(2)	0(1)	16(1)	-3(1)
C(85)	19(2)	32(2)	35(2)	4(1)	9(1)	6(1)
C(86)	23(2)	23(2)	22(2)	3(1)	2(1)	3(1)
C(87)	15(1)	17(1)	17(1)	-4(1)	-1(1)	-6(1)
C(88)	20(2)	23(2)	19(2)	-2(1)	-2(1)	-4(1)
C(89)	31(2)	30(2)	18(2)	6(1)	-6(1)	-12(1)
C(90)	22(2)	49(2)	18(2)	-1(1)	2(1)	-21(2)
C(91)	14(2)	44(2)	25(2)	-13(1)	6(1)	-8(1)
C(92)	18(2)	22(2)	20(2)	-5(1)	0(1)	-4(1)

C(93)	20(2)	13(1)	15(1)	5(1)	5(1)	-1(1)
C(94)	18(2)	18(1)	27(2)	2(1)	5(1)	0(1)
C(95)	24(2)	25(2)	34(2)	4(1)	12(1)	7(1)
C(96)	39(2)	15(1)	25(2)	0(1)	13(1)	7(1)
C(97)	36(2)	16(1)	16(2)	2(1)	0(1)	-2(1)
C(98)	19(2)	17(1)	17(2)	2(1)	1(1)	2(1)

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ([$PhBP_3$]Fe)$_2$(μ-N)·2 THF.

	x	y	z	U(eq)
H(1A)	6645	-194	4689	68
H(1B)	6534	823	4984	68
H(2A)	7476	-262	5165	52
H(2B)	7426	873	5344	52
H(3A)	7948	1400	4710	74
H(3B)	8103	257	4615	74
H(4A)	7537	1219	3904	87
H(4B)	7393	71	3992	87
H(5A)	7893	7716	10216	105
H(5B)	8213	8067	9725	105
H(6A)	7334	7841	9322	108
H(6B)	7021	8118	9833	108
H(7A)	6936	9581	9468	126
H(7B)	7461	9393	9124	126
H(8A)	7987	10265	9685	82
H(8B)	7490	10296	10071	82
H(10)	2975	831	3570	20
H(11)	3837	793	4075	22
H(12)	3983	1780	4811	24
H(13)	3244	2826	5030	23
H(14)	2386	2854	4521	19
H(15A)	2040	3282	3244	17
H(15B)	1874	3446	3821	17
H(16A)	1901	481	3220	17
H(16B)	2338	1227	2989	17
H(17A)	1438	1919	4301	18
H(17B)	1629	818	4178	18
H(19)	79	4539	3287	24
H(20)	-265	5649	3864	29
H(21)	179	5797	4699	31
H(22)	930	4748	4969	35
H(23)	1282	3638	4394	26
H(25)	616	3783	2207	20
H(26)	642	5163	1671	28
H(27)	1149	6575	1964	27
H(28)	1654	6569	2781	31
H(29)	1625	5193	3312	26
H(31)	2507	2565	2666	19
H(32)	2933	3686	2137	24
H(33)	2472	4124	1339	31
H(34)	1586	3441	1066	32
H(35)	1145	2359	1599	25
H(37)	2108	678	1802	24
H(38)	2095	-764	1312	27
H(39)	1405	-1971	1413	29
H(40)	732	-1733	2001	31
H(41)	732	-272	2484	21
H(43)	1532	-564	3822	26

H(44)	1391	-2255	3696	34
H(45)	488	-2883	3473	33
H(46)	-292	-1808	3361	31
H(47)	-150	-104	3431	23
H(49)	-282	2292	3769	30
H(50)	-865	2620	4427	45
H(51)	-641	1996	5256	39
H(52)	170	1009	5422	35
H(53)	738	640	4762	26
H(55)	-2830	849	1337	24
H(56)	-3736	915	918	26
H(57)	-4009	2228	371	27
H(58)	-3337	3445	219	25
H(59)	-2420	3361	630	21
H(60A)	-2277	1446	2028	19
H(60B)	-2212	2617	2068	19
H(61A)	-1554	1025	823	19
H(61B)	-1784	456	1302	19
H(62A)	-1750	3610	1229	20
H(62B)	-1351	2935	908	20
H(64)	-1136	1049	3492	23
H(65)	-1222	-476	3889	28
H(66)	-1609	-1824	3413	26
H(67)	-1905	-1626	2538	29
H(68)	-1838	-90	2141	23
H(70)	-796	3314	3146	22
H(71)	-1032	4289	3835	30
H(72)	-1944	4225	4113	33
H(73)	-2639	3209	3682	30
H(74)	-2404	2208	3002	24
H(76)	-1172	-840	903	32
H(77)	-1110	-2552	1015	39
H(78)	-639	-3202	1768	36
H(79)	-266	-2150	2422	34
H(80)	-342	-434	2321	24
H(82)	-901	1522	392	27
H(83)	-258	1654	-231	30
H(84)	692	1212	-35	35
H(85)	998	642	796	34
H(86)	351	491	1416	27
H(88)	-832	5215	1227	25
H(89)	-265	5907	632	32
H(90)	482	5002	335	35
H(91)	681	3422	648	33
H(92)	147	2744	1272	24
H(94)	-1965	4271	1936	25
H(95)	-2187	5597	2447	32
H(96)	-1470	6504	2907	31
H(97)	-517	6042	2872	27
H(98)	-292	4685	2381	21